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(57) Abstract

A method of constructing a variant of a parent Termamyl-like α-amylase, which variant has α-amylase activity and at least one altered property as compared to the parent α-amylase, comprises i) analysing the structure of the parent Termamyl-like α-amylase to identify at least one amino acid residue or at least one structural part of the Termamyl-like α-amylase structure, which amino acid residue or structural part is believed to be of relevance for altering the property of the parent Termamyl-like α-amylase (as evaluated on the basis of structural or functional considerations), ii) constructing a Termamyl-like α-amylase variant, which as compared to the parent Termamyl-like α-amylase, has been modified in the amino acid residue or structural part identified in i) so as to alter the property, and iii) testing the resulting Termamyl-like α-amylase variant for the property in question.

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A METHOD OF DESIGNING ALPHA-AMYLASE MUTANTS WITH PREDETERMINED PROPERTIES

FIELD OF THE INVENTION

The present invention relates to a novel method of designing α-amylase mutants with predetermined properties, which method is based on the hitherto unknown three-dimensional structure of bacterial α-amylases.

BACKGROUND OF THE INVENTION

α-Amylases (α-1,4 glucan-4-glucanohydrolase, EC 3.2.1.1) constitute a group of enzymes which is capable of hydrolyzing starch and other linear and branched 1,4-glucosidic oligo- and polysaccharides. Almost all α-amylases studied have a few conserved regions with approximately the same length and spacing. One of these regions resembles the Ca2+ binding site of calmodulin and the others are thought to be necessary for the active centre and/or binding of the substrate.

While the amino acid sequence and thus primary structure of a large number of α-amylases are known, it has proved very difficult to determine the three-dimensional structure of all α-amylases. The three-dimensional structure can be determined by X-ray crystallographic analysis of α-amylase crystals, but it has proven difficult to obtain α-amylase crystals suitable for actually solving the structure.

Until now the three-dimensional structure of only a few α-amylases have been determined at high resolution. These include the structure of the *Aspergillus oryzae* TAKA α-amylase (Swift et al., 1991), the *Aspergillus niger* acid amylase (Brady et al, 1991), the structure of pig pancreatic α-amylase (Qian et al., 1993), and the barley alpha-amylase (Kadziola et al. 1994, Journal of Molecular Biology 239: 104-121, A.Kadziola, Thesis, Dept of Chemistry, U. of Copenhagen, Denmark). Furthermore, the three-dimensional structure of a *Bacillus circulans* cyclodextrin glycosyltransferase (CGTase) is known

(Klein et al., 1992) (Lawson et al., 1994). The CGTase catalyzes the same type of reactions as α-amylases and exhibits some structural resemblance with α-amylases.

Furthermore, crystallization and preliminary X-ray studies of *B. subtilis* α-amylases have been described (Chang et al. (1992) and Mizuno et al. (1993)). No final *B. subtilis* structure has been reported. Analogously, the preparation of *B. licheniformis* α-amylase crystals has been reported (Suzuki et al. (1990), but no subsequent report on X-ray crystallographic analysis or three-dimensional structure are available.

Several research teams have attempted to build three-dimensional structures on the basis of the above known α-amylase structures. For instance, Vihinen et al. (J. Biochem. 107, 267-272, 1990), disclose the modelling (or computer simulation) of a three-dimensional structure of the *Bacillus stearothermophilus* α-amylase on the basis of the TAKA amylase structure. The model was used to investigate hypothetical structural consequences of various site-directed mutations of the *B. stearothermophilus* α-amylase. E.A. MacGregor (1987) predicts the presence of α-helices and ß-barrels in α-amylases from different sources, including barley, pig pancreas and *Bacillus amyloliquefaciens* on the basis of the known structure of the *A. oryzae* TAKA α-amylase and secondary structure predicting algorithms. Furthermore, the possible loops and subsites which may be found to be present in, e.g., the *B. amyloliquefaciens* α-amylase are predicted (based on a comparison with the *A. oryzae* sequence and structure).

A.E. MacGregor (Starch/Stärke 45 (1993), No. 7, p. 232-237) presents a review of the relationship between the structure and activity of α-amylase related enzymes.

Hitherto, no three-dimensional structure has been available for the industrially important *Bacillus* α-amylases (which in the present context are termed "Termamyl-like α-amylases"),

including the *B. licheniformis*, the *B. amyloliquefaciens*, and the *B. stearothermophilus* α-amylase.

BRIEF DISCLOSURE OF THE INVENTION

The three-dimensional structure of a Termamyl-like bacterial α-amylase has now been elucidated. On the basis of an analysis of said structure it is possible to identify structural parts or specific amino acid residues which from structural or functional considerations appear to be important for conferring the various properties to the Termamyl-like α-amylases. Furthermore, when comparing the Termamyl-like α-amylase structure with known structures of the fungal and mammalian α-amylases mentioned above, it has been found that some similarities exist between the structures, but also that some striking, and not previously predicted structural differences between the α-amylases exist. The present invention is based on these findings.

Accordingly, in a first aspect the invention relates to a method of constructing a variant of a parent Termamyl-like α-amylase, which variant has α-amylase activity and at least one altered property as compared to said parent α-amylase, which method comprises

i) analysing the structure of the Termamyl-like α-amylase with a view to identifying at least one amino acid residue or at least one structural part of the Termamyl-like α-amylase structure, which amino acid residue or structural part is believed to be of relevance for altering said property of the parent Termamyl-like α-amylase (as evaluated on the basis of structural or functional considerations),

ii) constructing a Termamyl-like α-amylase variant, which as compared to the parent Termamyl-like α-amylase, has been modified in the amino acid residue or structural part identified in i) so as to alter said property, and

iii) testing the resulting Termamyl-like α-amylase variant for said property.

In a second aspect the present invention relates to a method of constructing a variant of a parent Termamyl-like α-amylase, which variant has α-amylase activity and one or more altered properties as compared to said parent α-amylase, which method comprises

i) comparing the three-dimensional structure of the Termamyl-like α-amylase with the structure of a non-Termamyl-like α-amylase,

ii) identifying a part of the Termamyl-like α-amylase structure which is different from the non-Termamyl-like α-amylase structure, and

iii) modifying the part of the Termamyl-like α-amylase identified in ii) whereby a Termamyl-like α-amylase variant is obtained, one or more properties of which differ from the parent Termamyl-like α-amylase.

In a third aspect the invention relates to a method of constructing a variant of a parent non-Termamyl-like α-amylase, which variant has α-amylase activity and one or more altered properties as compared to said parent α-amylase, which method comprises

i) comparing the three-dimensional structure of the non-Termamyl-like α-amylase with the structure of a Termamyl-like α-amylase,

ii) identifying a part of the non-Termamyl-like α-amylase structure which is different from the Termamyl-like α-amylase structure, and

iii) modifying the part of the non-Termamyl-like α-amylase identified in ii) whereby a non-Termamyl-like α-amylase variant is obtained, one or more properties of which differ from the parent Termamyl-like α-amylase.

The property which may be altered by the above methods of the present invention may, e.g., be substrate specificity,

substrate binding, substrate cleavage pattern, temperature stability, pH dependent activity, pH dependent stability (especially increased stability at low (e.g. pH<6, in particular pH<5) or high (e.g. pH>9) pH values), stability towards oxidation, Ca^{2+}-dependency, specific activity, and other properties of interest. For instance, the alteration may result in a variant which, as compared to the parent Termamyl-like α-amylase, has an increased specific activity at a given pH and/or an altered substrate specificity.

In still further aspects the invention relates to variants of a Termamyl-like α-amylase, DNA encoding such variants and methods of preparing the variants. Finally, the invention relates to the use of the variants for various industrial purposes.

DETAILED DISCLOSURE OF THE INVENTION

<u>The Termamyl-like α-amylase</u>

It is well known that a number of alpha-amylases produced by *Bacillus* spp. are highly homologous on the amino acid level. For instance, the *B. licheniformis* α-amylase comprising the amino acid sequence shown in SEQ ID No. 2 (commercially available as Termamyl®) has been found to be about 89% homologous with the *B. amyloliquefaciens* α-amylase comprising the amino acid sequence shown in SEQ ID No. 4 and about 79% homologous with the *B. stearothermophilus* α-amylase comprising the amino acid sequence shown in SEQ ID No. 6. Further homologous α-amylases include an α-amylase derived from a strain of the *Bacillus* sp. NCIB 12289, NCIB 12512, NCIB 12513 or DSM 9375, all of which are described in detail in WO 95/26397, and the α-amylase described by Tsukamoto et al., 1988, Biochemical and Biophysical Research Communications, Vol. 151, No. 1. Still other homologous α-amylases include the α-amylase produced by the *B. licheniformis* described in EP 252 666 (ATCC 27811), and the α-amylases identified in WO 91/00353 and WO 94/18314. Other commercial Termamyl-like *B.*

licheniformis α-amylases are Optitherm® and Takatherm® (available from Solvay), Maxamyl® (available from Gist-brocades/Genencor), Spezym AA® (available from Genencor), and Keistase® (available from Daiwa).

Because of the substantial homology found between these α-amylases, they are considered to belong to the same class of α-amylases, namely the class of "Termamyl-like α-amylases".

Accordingly, in the present context, the term "Termamyl-like α-amylase" is intended to indicate an α-amylase which, on the amino acid level, exhibits a substantial homology to Termamyl®, i.e. the *B. licheniformis* α-amylase SEQ ID NO 2. In other words, a Termamyl-like α-amylase is an α-amylase, which has the amino acid sequence shown in SEQ ID No. 2, 4 or 6 herein, or the amino acid sequence shown in SEQ ID NO 1 or 2 of WO 95/26397 or in Tsukamoto et al., 1988, or i) which displays at least 60%, such as at least 70%, e.g. at least 75%, or at least 80%, e.g. at least 85%, at least 90% or at least 95% homology with at least one of said amino acid sequences and/or ii) displays immunological cross-reactivity with an antibody raised against at least one of said α-amylases, and/or iii) is encoded by a DNA sequence which hybridizes to the DNA sequences encoding the above specified α-amylases which are apparent from SEQ ID Nos. 1, 3 and 5 of the present application, and SEQ ID NO 4 and 5 of WO 95/26397, respectively.

In connection with property i) the "homology" may be determined by use of any conventional algorithm, preferably by use of the GAP progamme from the GCG package version 7.3 (June 1993) using default values for GAP penalties (Genetic Computer Group (1991) Programme Manual for the GCG Package, version 7, 575 Science Drive, Madison, Wisconsin, USA 53711).

Property ii) of the α-amylase, i.e. the immunological cross reactivity, may be assayed using an antibody raised against or reactive with at least one epitope of the relevant Termamyl-like α-amylase. The antibody, which may either be monoclonal or

polyclonal, may be produced by methods known in the art, e.g. as described by Hudson et al., 1989. The immunological cross-reactivity may be determined using assays known in the art, examples of which are Western Blotting or radial immunodiffusion assay, e.g. as described by Hudson et al., 1989. In this respect, immunological cross-reactivity between the α-amylases having the amino acid sequences SEQ ID Nos. 2, 4 and 6, respectively, has been found.

The oligonucleotide probe used in the characterization of the Termamyl-like α-amylase in accordance with property iii) above may suitably be prepared on the basis of the full or partial nucleotide or amino acid sequence of the α-amylase in question. Suitable conditions for testing hybridization involve presoaking in 5xSSC and prehybridizing for 1h at ~40°C in a solution of 20% formamide, 5xDenhardt's solution, 50mM sodium phosphate, pH 6.8, and 50μg of denatured sonicated calf thymus DNA, followed by hybridization in the same solution supplemented with 100μM ATP for 18h at ~40°C, or other methods described by e.g. Sambrook et al., 1989.

In the present context, "derived from" is intended not only to indicate an α-amylase produced or producible by a strain of the organism in question, but also an α-amylase encoded by a DNA sequence isolated from such strain and produced in a host organism transformed with said DNA sequence. Finally, the term is intended to indicate an α-amylase which is encoded by a DNA sequence of synthetic and/or cDNA origin and which has the identifying characteristics of the α-amylase in question. The term is also intended to indicate that the parent α-amylase may be a variant of a naturally occurring α-amylase, i.e. a variant which is the result of a modification (insertion, substitution, deletion) of one or more amino acid residues of the naturally occurring α-amylase.

Parent hybrid α-amylases

The parent α-amylase (being a Termamyl-like or non-Termamyl-like α-amylase) may be a hybrid α-amylase, i.e. an α-amylase which comprises a combination of partial amino acid sequences derived from at least two α-amylases.

The parent hybrid α-amylase may be one which on the basis of amino acid homology and/or immunological cross-reactivity and/or DNA hybridization (as defined above) can be determined to belong to the Termamyl-like α-amylase family. In this case, the hybrid α-amylase is typically composed of at least one part of a Termamyl-like α-amylase and part(s) of one or more other α-amylases selected from Termamyl-like α-amylases or non-Termamyl-like α-amylases of microbial (bacterial or fungal) and/or mammalian origin.

Thus, the parent hybrid α-amylase may comprise a combination of at least two Termamyl-like α-amylases, or of at least one Termamyl-like and at least one non-Termamyl-like bacterial α-amylase, or of at least one Termamyl-like and at least one fungal α-amylase. For instance, the parent α-amylase comprises a C-terminal part of an α-amylase derived from a strain of *B. licheniformis* and a N-terminal part of an α-amylase derived from a strain of *B. amyloliquefaciens* or from a strain of *B. stearothermophilus*. For instance, the parent α-amylase comprises at least 430 amino acid residues of the C-terminal part of the *B. licheniformis* α-amylase, and may, e.g. comprise a) an amino acid segment corresponding to the 37 N-terminal amino acid residues of the *B. amyloliquefaciens* α-amylase having the amino acid sequence shown in SEQ ID No. 4 and an amino acid segment corresponding to the 445 C-terminal amino acid residues of the *B. licheniformis* α-amylase having the amino acid sequence shown in SEQ ID No. 2, or b) an amino acid segment corresponding to the 68 N-terminal amino acid residues of the *B. stearothermophilus* α-amylase having the amino acid sequence shown in SEQ ID No. 6 and an amino acid segment corresponding to the 415 C-terminal amino acid residues of the

B. licheniformis α-amylase having the amino acid sequence shown in SEQ ID No. 2.

Analogously, the parent hybrid α-amylase may belong to a non-Termamyl-like α-amylase family, e.g. the Fungamyl-like α-amylase family. In that case the hybrid may comprise at least one part of an α-amylase belonging to the non-Termamyl-like α-amylase family in combination with one or more parts derived from other α-amylases.

The three-dimensional Termamyl-like α-amylase structure

The Termamyl-like α-amylase which was used to elucidate the three-dimensional structure forming the basis for the present invention consists of the 300 N-terminal amino acids of the *B. amyloliquefaciens* α-amylase (with the amino acid sequence shown in SEQ ID No. 4) and amino acids 301-483 of the C-terminal end of the *B. licheniformis* α-amylase with the amino acid sequence SEQ ID No. 2. The bacterial α-amylase belongs to the "Termamyl-like α-amylase family" and the present structure is believed to be representative for the structure of any Termamyl-like α-amylase.

The structure of the α-amylase was solved in accordance with the principle for X-ray crystallographic methods given in "X-Ray Structure Determination", Stout, G.K. and Jensen, L.H., John Wiley & Sons, inc. NY, 1989. The structural coordinates for the solved crystal structure of the α-amylase at 2.2 Å resolution using the isomorphous replacement method are given in a standard PDB format (Brookhaven Protein Data Base) in Appendix 1. It is to be understood that Appendix 1 forms part of the present application.

Amino acid residues of the enzyme are identified by three-letter amino acid code (capitalized letters).

The α-amylase structure is made up of three globular domains ordered A, B, and C with respect to sequence, which lie

approximately along a line in the order B, A, C. The domains can be defined as being residues 1-103 and 206-395 for domain A, residues 104-205 for domain B, and residues 396-483 for domain C, the numbers referring to the *B. licheniformis* α-amylase. This gives rise to an elongated molecule, the longest axis being about 85Å. The widest point perpendicular to this axis is approximately 50Å and spans the central A domain. The active site residues of the *B. licheniformis* α-amylase (SEQ ID NO 2) are D323, D231 and E261.

Domain A

Domain A is the largest domain and contains the active site (comprised of a cluster of three amino acid residues placed at the bottom of a deep cleft in the enzyme's surface). Domain A of all known α-amylase structures have the same overall fold, viz. the (beta/alpha)8 barrel with 8 central beta strands (number 1-8) and 8 flanking α-helices. The β-barrel is defined by McGregor *op. cit.* The C-terminal end of Beta strand 1 is connected to helix 1 by a loop denoted loop 1 and an identical pattern is found for the other loops. These loops show some variation in size and some can be quite extensive.

The 8 central Beta-strands in the (beta/alpha)8 barrel superimpose well between the various known α-amylase structures, and this part of the structure, including the close surroundings of the active site located at the c-terminal end of the beta-strands, show high similarity between the different amylases.

The loops connecting beta-strands and alpha helices display high variations between alpha amylases. These loops constitute the structural context of the active site and the majority of the contacts to the substrate is found among residues located in these loops. Such important characteristics as substrate specificity, substrate binding, pH/activity profile, starch cleavage pattern are determined by the amino acids and the positions of same in these loops.

The substantial differences between the Fungamyl-like α-amylase structure and the structure of the Termamyl-like α-amylase disclosed herein which are found in loops 1, 2, 3, and 8 are visualized in the Figures.

Domain B

The Termamyl-like α-amylase structure has been found to comprise a special domain structure in the A domain's loop3, also called domain B. The structure of the Termamyl-like α-amylase B domain has never been seen before in any of the known α-amylase or (β/alpha)8-barrel proteins.

The domain B structure is a very compact domain having a very high number of charged residues. The B domain arises as an extension of the loop between strand 3 and helix 3 of domain A (shown in Fig. 7) and contains a 5 stranded antiparallel β-sheet structure containing at least one long loop structure and having the connectivity -1, +3, -1X, +2 (Richardson, 1981, Adv. Protein Chem. 34, 167-339).

The first four strands of the B domain form two hairpin loops which twist around each other like a pair of crossed fingers (right-hand twist). The mainchain folds into a ß-strand which connects two small ß-sheet structures. After making one turn in one sheet it folds back and makes up a two stranded sheet in contact with domain A and an internal hole in the α-amylase structure. Then the mainchain folds up to a small sheet structure nearly perpendicular to the first two sheets. Before entering the helix 3 on top of the ß-strand 3, the approximately 24 last amino acids in domain B form two calcium binding sites in the contact region to domain A.

Domain B is connected with domain A by two peptide stretches, which divide the domain-domain contact areas into two. Domain B is in contact with Domain A by a calcium binding region and an internally buried hole containing waters. Many types of molecular contacts are present. Ionic interacting between acid

and basic amino acids are possible, these interactions are very important for the general stability at high pH and for keeping the Calcium binding sites intact.

Domain C

Domain C is the C-terminal part of the protein consisting of amino acids 394-483. Domain C is composed entirely of β-strands which forms a single 8-stranded sheet structure, which folds back on itself, and thus may be described as a β-sandwich structure. The connectivity is +1,+1, +5, -3, +1, +1, -3 although strands 6 and 7 are only loosely connected. One part of the β-sheet forms the interface to domain A.

Ca-binding and Na-binding sites

The structure of the Termamyl-like α-amylase is remarkable in that it exhibits four calcium-binding sites and one sodium-binding site. In other words four calcium ions and one sodium ion are found to be present in the structure, although one of the calcium ions displays very weak coordination. Two of the calcium ions form part of a linear cluster of three ions, the central ion being attributed to sodium, which lie at the junction of the A and B domains.

The coordinating residues for the calcium ions between the A and B domain are as follows (using the Pdb file nomenclature for amino acid residues and atoms in the Pdb file found in Appendix 1 herein): For the calcium ion nearest to the active site (IUM 502 in the pdb file), the backbone carbonyls from His235 and Asp194, the sidechain atom OD1 from residues Asp194, Asn102 and Asp200, and one water molecule WAT X3 (atom OW7). For the sodium ion (IUM 505), the binding site includes atom OD2 from Asp194, Asp200, Asp183 and Asp159, and a backbone carbonyl from Val201. The coordinates for the other calcium ion between domain A and B are (IUM 501) : atom OD2 from Asp204 and Asp159, backbone carbonyl from Asp183 and Ala181, atom OD1 from Asp202, and one water molecule WAT X7 (atom OW7).

One calcium ion is located between the A and C domain, another is located in the C domain. The first mentioned calcium ion, which is also the one best coordinated (IUM 503) includes a carbonyl backbone from Gly300, Tyr302 and His406, atom OD2/OD1 from Asp430, atom OD1 from Asp407, and one water molecule WAT X6 (atom OW7). The other and very weakly coordinated calcium site (IUM 504) comprises 4 water molecules WAT X21 (atom OW8), X6 (atom OW6), X9 (atom OW0) and X28 (atom OW8), OE1/OE2 from Glu447 and OD1 from Asn444.

Substrate-binding site

Without being limited to any theory it is presently believed that favourable interactions between a substrate molecule and the enzyme (such as hydrogen bonds and/or strong electrostatic interaction) are found within a sphere of 4Å of the substrate, when bound to the enzyme. The following residues of the *B. licheniformis* α-amylase having the amino acid sequence shown in SEQ ID No. 2 are contemplated to be within a distance of 4 Å of the substrate and thus believed to be involved in interactions with the substrate:
Trp13, Tyr14, Asn17, Asp18, Ser50, Gln51, Ala52, Asp53, Val54, Gly55, Tyr56, Lys70, Arg74, Lys76, Val102, His105, Gly107, Gly108, Ala109, Trp138, Thr163, Asp164, Trp165, Asn172, Glu189, Tyr193, Leu196, Met197, Tyr198, Ala199, Arg229, Asp231, Ala232, Lys234, His235, Glu261, Trp263, His327, Asp328, Gln333, Ser334, and Leu335.

The amino acid residues of another Termamyl-like α-amylase, which are contemplated to be within a distance of 4Å of the substrate, may easily be identified by aligning the amino acid sequence SEQ ID NO 2 with that of the other Termamyl-like α-amylase and thereby identifying the positions equivalent to those identified above.

Generality of structure

Because of the high homology between the various Termamyl-like α-amylases, the solved structure defined by the coordinates of Appendix 1 is believed to be representative for the structure of all Termamyl-like α-amylases. A model structure of other Termamyl-like α-amylases may easily be built on the basis of the coordinates given in Appendix 1 adapted to the α-amylase in question by use of an alignment betweeen the respective amino acid sequences. The creation of a model structure is exemplified in Example 1.

The above identified structurally characteristic parts of the Termamyl-like α-amylase structure (Ca-binding site, substrate binding site, loops, etc.) may easily be identified in other Termamyl-like α-amylases on the basis of a model (or solved) structure of the relevant Termamyl-like α-amylase or simply on the basis of an alignment between the amino acid sequence of the Termamyl-like α-amylase in question with that of the *B. lichenformis* α-amylase used herein for identifying the amino acid residues of the respective structural elements.

Furthermore, in connection with Termamyl-like variants of the invention, which are defined by modification of specific amino acid residues of a specific Termamyl-like α-amylase, it will be understood that variants of another Termamyl-like α-amylase modified in an equivalent position (as determined from the best possible amino acid sequence alignment between the respective sequences) are intended to be covered as well. Thus, irrespective of whether an amino acid residue is identified herein for the purpose of defining a structural part of a given α-amylase or used for identifying a variant of the α-amylase, this amino acid residue shall be considered as representing the equivalent amino acid residue of any other Termamyl-like α-amylase.

Methods of the invention for design of novel α-amylase variants

In the methods according to the first, second and third aspects of the invention the terms "structure of a Termamyl-like α-amylase" and "Termamyl-like α-amylase structure" are intended to indicate the solved structure defined by the coordinates presented in Appendix 1 or a model structure of a given Termamyl-like α-amylase (such as the *B. licheniformis* α-amylase) built on the basis of the solved structure.

In most cases the parent Termamyl-like α-amylase to be modified in accordance with the present invention is different from the α-amylase which was actually used for solving the structure (Appendix 1). This means that the amino acid residue(s) or structural part(s) identified in the solved structure (Appendix 1) in step i) of the method according to the first, second or third aspect of the invention must be translated into the corresponding amino acid residue(s) or structural part(s) of the parent Termamyl-like α-amylase in question. The "translation" is conveniently performed on the basis of an amino acid sequence alignment between the amino acid sequence of the Termamyl-like α-amylase used for solving the structure and the amino acid sequence of the parent Termamyl-like α-amylase in question.

The analysis or comparison performed in step i) of the method according to the first, second and third aspect, respectively, of the invention may be performed by use of any suitable computer programme capable of analysing and/or comparing protein structures, e.g. the computer programme Insight, available from Biosym Technologies, Inc. For instance, the basic principle of structure comparison is that the three-dimensional structures to be compared are superimposed on the basis of an alignment of secondary structure elements (such as the central 8 β-strands in the barrel) and the parts differing between the structures can subsequently easily be identified from the superimposed structure.

The structural part which is identified in step i) of the methods of the first, second and third aspects of the invention may be composed of one amino acid residue. However, normally the structural part comprises more than one amino acid residue, typically constituting one of the above parts of the Termamyl-like α-amylase structure such as one of the A, B, or C domains, an interface between any of these domains, a calcium binding site, a loop structure, the substrate binding site, or the like.

In the present context the term "structural or functional considerations" is intended to indicate that modifications are made on the basis of an analysis of the relevant structure or structural part and its contemplated impact on the function of the enzyme. Thus, an analysis of the structures of the various α-amylases, which until now has been elucidated, optionally in combination with an analysis of the functional differences between these α-amylases, may be used for assigning certain properties of the α-amylases to certain parts of the α-amylase structure or to contemplate such relationship. For instance, differences in the pattern or structure of loops surrounding the active site may result in differences in access to the active site of the substrate and thus differences in substrate specificity and/or cleavage pattern. Furthermore, parts of a Termamyl-like α-amylase involved in or contemplated to be involved in substrate binding (and thus e.g. specificity/cleavage pattern), calcium or sodium ion binding (e.g. of importance for the Calcium-dependency of the enzyme), and the like has been identified (*vide infra*).

The modification of an amino acid residue or structural part is typically accomplished by suitable modifications of a DNA sequence encoding the parent enzyme in question. The term "modified" as used in step ii) in the method according to the first aspect of the invention is intended to have the following meaning: When used in relation to an amino acid residue the term is intended to mean replacement of the amino acid residue in question with another amino acid residue. When used in

relation to a structural part, the term is intended to mean replacement of one or more amino acid residues of said structural part, addition of one or more amino acid residues to said part, or deletion of one or more amino acid residues of said structural part.

The construction of the variant of interest is accomplished by cultivating a microorganism comprising a DNA sequence encoding the variant under conditions which are conducive for producing the variant, and optionally subsequently recovering the variant from the resulting culture broth. This is described in detail further below.

First aspect of the invention
In a preferred embodiment of the method according to the first aspect of the invention the property of the parent enzyme to be modified is selected from calcium dependency, substrate binding, cleavage pattern, pH dependent activity and the like. Specific examples of how to change these properties of a parent Termamyl-like α-amylase are given further below.

In another preferred embodiment the parent Termamyl-like α-amylase to be modified is a *B. licheniformis* α-amylase.

Second and third aspects of the invention
One important advantage of the methods according to the second and third aspects of the present invention is that it is possible to adapt the structure (or a structural part) of a Termamyl-like α-amylase to the structure (or structural part) of a non-Termamyl-like α-amylase and *vide versa*. For instance, having identified a loop structure of the non-Termamyl-like α-amylase which is believed to be responsible for or contributing to a particular property of the non-Termamyl-like α-amylase it is possible to replace the corresponding structure of the Termamyl-like α-amylase with said non-Termamyl-like α-amylase structure - or if no corresponding structure exists in the Termamyl-like α-amylase - to insert the structure into the Termamyl-like α-amylase in such a manner that the resulting

variant Termamyl-like α-amylase, as far as the relevant part is concerned, resembles the corresponding part of the non-Termamyl-like α-amylase. When two or more parts of the structure of the parent Termamyl-like α-amylase are modified so as to resemble the corresponding parts of the non-Termamyl-like α-amylase it is possible to increase the resemblance to the non-Termamyl-like α-amylase of the Termamyl-like α-amylase variant and thus to alter the properties of said variant in the direction of those of said non-Termamyl-like α-amylase. Loop modifications are discussed in much further detail further below.

Typically, the modification to be performed in step iii) of the method according to the second aspect of the invention is accomplished by deleting one or more amino acid residues of the part of the Termamyl-like α-amylase to be modified so as to adapt the structure of said part of the parent α-amylase to the corresponding part of the non-Termamyl-like α-amylase; by replacing one or more amino acid residues of the part of the Termamyl-like α-amylase to be modified with the amino acid residues occupying corresponding positions in the non-Termamyl-like α-amylase; or by insertion of one or more amino acid residues present in the non-Termamyl-like α-amylase into a corresponding position in the Termamyl-like α-amylase. For the method according to the third aspect the modification is to be understood analogously, performed on the non-Termamyl-like parent α-amylase rather than the Termamyl-like α-amylase.

In step ii) of the method according to the second or third aspect of the invention the part of the structure to be identified is preferably one which in the folded enzyme is believed to be in contact with the substrate (cf the disclosure above in the section entitled "Substrate-binding site) or involved in substrate specificity and/or cleavage pattern, and/or one which is in contact with one of the calcium or sodium ions and/or one, which is contributing to the pH or temperature profile of the enzyme, or one which otherwise, from structural or functional considerations, is contemplated to be

responsible for differences in one or more properties of the Termamyl-like and non-Termamyl-like α-amylase.

Non-Termamyl-like α-amylase

The non-Termamyl-like α-amylase with which the comparison is made in step i) of the method of the second aspect of the invention and which is the parent α-amylase in the method of the third aspect of the invention, may be any α-amylase, which does not belong to the family of Termamyl-like α-amylases (as defined above) and, which as a consequence thereof, has a different three-dimensional structure. Furthermore, the non-Termamyl-like α-amylase should be one which has, at the time that the method is performed, an elucidated or contemplated three-dimensional structure.

The non-Termamyl-like α-amylase may, e.g., be a fungal α-amylase, a mammalian or a plant α-amylase or a bacterial α-amylase (different from a Termamyl-like α-amylase). Specific examples of such α-amylases include the *Aspergillus oryzae* TAKA α-amylase, the *A. niger* acid α-amylase, the *Bacillus subtilis* α-amylase, the porcine pancreatic α-amylase and a barley α-amylase. All of these α-amylases have elucidated structures which are clearly different from the structure of the Termamyl-like α-amylase shown herein.

The fungal α-amylases mentioned above, i.e. derived from *A. niger* and *A. oryzae*, are highly homologous on the amino acid level and generally considered to belong to the same family of α-amylases. In the present disclosure, this family is termed "Fungamyl-like α-amylase" and intends to indicate an α-amylase which exhibits a high homology, i.e. more than 70%, such as 80% homologous (as defined herein) to the fungal α-amylase derived from *Aspergillus oryzae*, commercially available as Fungamyl®, and the *A. niger* α-amylase.

From the enclosed illustrations of the α-amylase structure of a Termamyl-like α-amylase and a comparison of said structure with the structure of a Fungamyl-like α-amylase it is evident

that major differences exist between the two structures. In the method of the invention it is of particular interest to modify parts of the parent Termamyl-like α-amylase, which belong to a region with large differences to the Fungamyl-like α-amylase. In particular, it is of interest to modify the parent Termamyl-like α-amylase in one or more of the following loops: loop 1, loop 2, loop 3 and/or loop 8 of the parent α-amylase.

In the method of the third aspect of the invention it is of particular interest to modify loop 1, loop 2, loop 3 and/or loop 8 of the parent non-Termamyl-like α-amylase to a closer ressemblance to the similar loops of a Termamyl-like α-amylase, such as Termamyl.

In the following specific types of variants are described which have been designed by use of the method of the invention.

Loop modifications

In order to change the substrate specificity of the parent α-amylase to be modified it is relevant to consider loop modifications. For instance changing one or more of the loop structures of the Termamyl-like α-amylase into a closer ressemblance with the corresponding loop structure(s) of a non-Termamyl-like α-amylase (such as a Fungamyl-like α-amylase) it is contemplated that it is possible to change the substrate specificity in the direction of that of the non-Termamyl α-amylase. In the following different types of loop modifications of interest are listed. It will be understood that the variants may have other changed properties in addition to the modified substrate specificity. It will be understood that the following modifications identified for a specific Termamyl-like α-amylase are intended to include corresponding modifications in other equivalent positions of other Termamyl-like α-amylases. Furthermore, it will be understood that, normally, the loop modification will comprise replacement of an entire loop structure or a substantial part thereof in, e.g., the Termamyl-

like α-amylase, with the corresponding loop structure (or substantial part thereof) in a non-Termamyl-like α-amylase.

Loop2 modifications

In one embodiment the invention relates to a variant of a parent Termamyl-like α-amylase, in which variant at least one amino acid residue of the parent α-amylase, which is/are present in a fragment corresponding to the amino acid fragment 44-57 of the amino acid sequence of SEQ ID No. 4, i.e. loop 2, has been deleted or replaced with one or more amino acid residues which is/are present in a fragment corresponding to the amino acid fragment 66-84 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has been added using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α-amylase as a template.

The amino acid sequence shown in SEQ ID No. 10 is the amino acid sequence of the *A. oryzae* α-amylase, i.e. a Fungamyl-like α-amylase. It will be understood that amino acid residues or fragments found in corresponding positions in other α-amylases, in particular Fungamyl-like α-amylases, may be used as a template for the construction of the variant according to the invention. The corresponding part in other homologous α-amylases may easily be identified on the basis of a comparison of the amino acid sequences and/or three-dimensional structures of the respective α-amylases.

For instance, the variant may be one, which, when the amino acid sequence of the variant is aligned most closely with the amino acid sequence of the said parent α-amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No 4, the said region having at least 80% such as at least 90% sequence homology with the part of SEQ ID No 10 extending from residue Z to residue V of SEQ ID No 10, wherein
X is the amino acid residue occupying position 44, 45, 46, 47 or 48 of SEQ ID No. 4,

Y is the amino acid residue occupying position 51, 52, 53, 54, 55, 56 or 57 of SEQ ID No. 4,
Z is the amino acid residue occupying position 66, 67, 68, 69 or 70 of SEQ ID No. 10, and
V is the amino acid residue occupying position 78, 79, 80, 81, 82, 83 or 84 of SEQ ID No. 10.

In other words, the variant may be one in which an amino acid fragment X-Y of the parent α-amylase, which corresponds to or is within the amino acid fragment 44-57 of SEQ ID No. 4, has been replaced with an amino acid fragment Z-V, which corresponds to or is within the amino acid fragment 66-84 of the amino acid sequence shown in SEQ ID No. 10, in X, Y, Z and V have the meaning indicated above.

A specific example of a variant according to this embodiment is a variant of a parent Termamyl-like α-amylase, in which the amino acid fragment of the parent α-amylase, which corresponds to amino acid residues 48-51 of SEQ ID No. 4, has been replaced with an amino acid fragment corresponding to amino acid residues 70-78 of the amino acid sequence shown in SEQ ID No. 10.

Loop 3 modifications - limited alteration

In another embodiment the invention relates to a variant of a parent Termamyl-like α-amylase, in which variant at least one of the amino acid residues of the parent α-amylase, which is/are present in an amino acid fragment corresponding to the amino acid fragment 195-202 of the amino acid sequence of SEQ ID No. 4, has been deleted or replaced with one or more of the amino acid residues which is/are present in an amino acid fragment corresponding to the amino acid fragment 165-177 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has been added using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α-amylase as a template.

For instance, the variant may be one in which an amino acid fragment X-Y of the parent α-amylase which corresponds to or is within the amino acid fragment 195-202 of SEQ ID No. 4, has been replaced by an amino acid fragment Z-V, which corresponds to or is within the amino acid fragment 165-177 of the amino acid sequence shown in SEQ ID No. 10, in which

X is an amino acid residue corresponding to the amino acid occupying position 195 or 196 of SEQ ID No. 4,

Y is an amino acid residue corresponding to the amino acid occupying position 198, 199, 200, 201, or 202 of SEQ ID No. 4,

Z is an amino acid residue corresponding to the amino acid occupying position 165 or 166 of SEQ ID No. 10, and

V is an amino acid residue corresponding to the amino acid occupying position 173, 174, 175, 176 or 177 of SEQ ID No. 10.

Expressed in another manner, the variant according to this aspect may be one, which, when the amino acid sequence of variant is aligned most closely with the amino acid sequence of the said parent Termamyl-like α-amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No 4, the said region having at least 80%, such as 90% sequence homology with the part of SEQ ID No 10 extending from residue Z to residue V of SEQ ID No 10, the meaning of X, Y, Z and V being as identified above.

A specific example of a variant according to this embodiment is a variant of a parent Termamyl-like α-amylase, in which the amino acid fragment of the parent α-amylase, which corresponds to amino acid residues 196-198 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino acid residues 166-173 of the amino acid sequence shown in SEQ ID No. 10.

Loop 3 modifications - complete domain B

In a further embodiment the invention relates to a variant of a parent Termamyl-like α-amylase, in which variant at least one of the amino acid residues of the parent α-amylase, which is/are present in a fragment corresponding to the amino acid fragment 117-185 of the amino acid sequence of SEQ ID No. 4, has/have been deleted or replaced with one or more of the amino acid residues, which is/are present in an amino acid fragment corresponding to the amino acid fragment 98-210 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has been added using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α-amylase as a template.

For instance, the variant may be one, in which an amino acid fragment X-Y of the parent α-amylase, which corresponds to or is within the amino acid fragment 117-185 of SEQ ID No. 4, has been replaced with an amino acid fragment Z-V, which corresponds to or is within the amino acid fragment 98-210 of the amino acid sequence shown in SEQ ID No. 10, in which variant

X is an amino acid residue corresponding to the amino acid occupying position 117, 118, 119, 120 or 121 of SEQ ID No. 4,

Y is an amino acid residue corresponding to the amino acid occupying position 181, 182, 183, 184 or 185 of SEQ ID No. 4,
Z is an amino acid residue corresponding to the amino acid occupying position 98, 99, 100, 101, 102 of SEQ ID No. 10, and

V is an amino acid residue corresponding to the amino acid occupying position 206, 207, 208, 209 or 210 of SEQ ID No. 10.

A specific example of a variant according to this embodiment is a variant of a parent α-amylase, in which an amino acid fragment of the parent α-amylase, which corresponds to amino acid residues 121-181 of SEQ ID No. 4, has been replaced with

the amino acid fragment corresponding to amino acid residues 102-206 of the amino acid sequence shown in SEQ ID No. 10.

In another embodiment the invention relates to a variant of a parent Termamyl-like α-amylase, in which variant at least one of the amino acid residues of the parent α-amylase, which is/are present in a fragment corresponding to the amino acid fragment 117-181 of the amino acid sequence of SEQ ID No. 4, has/have been deleted or replaced with one or more of the amino acid residues, which is/are present in an amino acid fragment corresponding to the amino acid fragment to 98-206 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has been added using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α-amylase as a template.

For instance, the variant may be one, in which the amino acid fragment X-Y of the parent α-amylase, which corresponds to or is within the amino acid fragment 117-177 if SEQ ID No. 4, has/have been replaced with an amino acid fragment Z-V, which corresponds to or is within the amino acid fragment 98-202 of the amino acid sequence shown in SEQ ID No. 10, in which variant

X is an amino acid residue corresponding to the amino acid occupying position 117, 118, 119, 120 or 121 of SEQ ID No. 4,

Y is an amino acid residue corresponding to the amino acid occupying position 174, 175, 176 or 177 of SEQ ID No. 4,

Z is an amino acid residue corresponding to the amino acid occupying position 98, 99, 100, 101, 102 of SEQ ID No. 10, and

V is an amino acid residue corresponding to the amino acid occupying position 199, 200, 201 or 202 of SEQ ID No. 10.

A specific example of a variant according to this embodiment of the invention is a variant, in which the amino acid fragment of

the parent α-amylase, which corresponds to amino acid residues 121-174 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino acid residues 102-199 of the amino acid sequence shown in SEQ ID No. 10.

Loop 1 modifications - minimal addition

In a further embodiment the present invention relates to a variant of a parent Termamyl-like α-amylase, in which variant at least one of the amino acid residues of the parent α-amylase, which is/are present in an amino acid fragment corresponding to the amino acid fragment 12-19 of the amino acid sequence of SEQ ID No. 4, has/have been deleted or replaced with one or more of the amino acid residues, which is/are present in an amino acid fragment which corresponds to the amino acid fragment 28-42 of SEQ ID No. 10, or in which one or more additional amino acid residues has/have been inserted using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α-amylase as a template.

For instance, the variant may be one, in which the amino acid fragment X-Y of the parent α-amylase, which corresponds to or is within the amino acid fragment 12-19 of SEQ ID No. 4, has/have been replaced with an amino acid fragment Z-V, which corresponds to or is within the amino acid fragment 28-42 of the amino acid sequence shown in SEQ ID No. 10, in which variant

X is an amino acid residue corresponding to the amino acid occupying position 12, 13 or 14 of SEQ ID No. 4,

Y is an amino acid residue corresponding to the amino acid occupying position 15, 16, 17, 18 or 19 of SEQ ID No. 4,

Z is an amino acid residue corresponding to the amino acid occupying position 28, 29, 30 , 31 or 32 of SEQ ID No. 10, and

V is an amino acid residue corresponding to the amino acid occupying position 38, 39, 40, 41 or 42 of SEQ ID No. 10.

A specific example of a variant according to this aspect of the invention is a variant, in which the amino acid fragment of the parent α-amylase, which corresponds to amino acid residues 14-15 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino acid residues 32-38 of the amino acid sequence shown in SEQ ID No. 10.

Loop 1 modifications - complete loop

In a further embodiment the invention relates to a variant of a parent Termamyl-like α-amylase, in which variant at least one of the amino acid residues of the parent α-amylase, which is present in a fragment corresponding to amino acid residues 7-23 of the amino acid sequence of SEQ ID No. 4, has/have been deleted or replaced with one or more amino acid residues, which is/are present in an amino acid fragment corresponding to amino acid residues 13-45 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has/have been inserted using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α-amylase as a template.

For instance, the variant may be one, in which the amino acid fragment X-Y of the parent α-amylase, which corresponds to or is within the amino acid fragment 7-23 of SEQ ID No. 4, has/have been replaced with an amino acid fragment Z-V, which corresponds to or is within the amino acid fragment 13-45 of the amino acid sequence shown in SEQ ID No. 10, in which variant

X is an amino acid residue corresponding to the amino acid occupying position 7 or 8 of SEQ ID No. 4,

Y is an amino acid residue corresponding to the amino acid occupying position 18, 19, 20, 21, 22 or 23 of SEQ ID No. 4,

Z is an amino acid residue corresponding to the amino acid occupying position 13 or 14 of SEQ ID No. 10, and

V is an amino acid residue corresponding to the amino acid occupying position 40, 41, 42, 43, 44 or 45 of SEQ ID No. 10.

A specific variant according to this embodiment is one, in which the amino acid fragment of the parent α-amylase, which corresponds to amino acid residues 8-18 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino acid residues 14-40 of the amino acid sequence shown in SEQ ID No. 10.

Loop 8 modifications

In a further embodiment the invention relates to a variant of a parent Termamyl-like α-amylase, in which variant at least one of the amino acid residues of the parent α-amylase, which is present in a fragment corresponding to amino acid residues 322-346 of the amino acid sequence of SEQ ID No. 2, has/have been deleted or replaced with one or more amino acid residues, which is/are present in an amino acid fragment corresponding to amino acid residues 291-313 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has/have been inserted using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α-amylase as a template.

For instance, the variant may be one, in which the amino acid fragment X-Y of the parent α-amylase, which corresponds to or is within the amino acid fragment 322-346 of SEQ ID No. 2, has/have been replaced with an amino acid fragment Z-V, which corresponds to or is within the amino acid fragment 291-313 of the amino acid sequence shown in SEQ ID No. 10, in which variant

X is an amino acid residue corresponding to the amino acid occupying position 322, 323, 324 or 325 of SEQ ID No. 2,

Y is an amino acid residue corresponding to the amino acid occupying position 343, 344, 345 or 346 of SEQ ID No. 2,

Z is an amino acid residue corresponding to the amino acid occupying position 291, 292, 293 or 294 of SEQ ID No. 10, and

V is an amino acid residue corresponding to the amino acid occupying position 310, 311, 312 or 313 of SEQ ID No. 10.

A specific variant according to this aspect of the invention is one, in which the amino acid fragment of the parent α-amylase, which corresponds to amino acid residues 325-345 of SEQ D No. 2, has been replaced with the amino acid fragment corresponding to amino acid residues 294-313 of the amino acid sequence shown in SEQ ID No. 10.

Ca^{2+} dependency

It is highly desirable to be able to decrease the Ca^{2+} dependency of a Termamyl-like α-amylase. Accordingly, in a further aspect the invention relates to a variant of a parent Termamyl-like α-amylase, which exhibits α-amylase activity and which has a decreased Ca^{2+} dependency as compared to the parent α-amylase. The decreased Ca^{2+} dependency has the functional result that the variant exhibits a satisfactory amylolytic activity in the presence of a lower concentration of calcium ion in the extraneous medium than is necessary for the parent enzyme and, for example, therefore is less sensitive than the parent to calcium ion-depleting conditions such as those obtained in media containing calcium-complexing agents (such as certain detergent builders).

The decreased Ca^{2+} dependency of the variant of the invention may advantageously be achieved by increasing the Ca^{2+} binding affinity of the parent Termamyl-like α-amylase, in other words the stronger the Ca^{2+} binding of the enzyme, the lower is the Ca^{2+} dependency.

It is presently believed that amino acid residues located within 10Å from a sodium or calcium ion are involved in or are of importance for the Ca^{2+} binding capability of the enzyme.

Accordingly, the variant according to this aspect of the invention is preferably one, which has been modified in one or more amino acid residues present within 10Å from a calcium and/or sodium ion identified in the three-dimensional Termamyl-like α-amylase structure in such a manner that the affinity of the α-amylase for calcium is increased.

The amino acid residues found within a distance of 10Å from the Ca^{2+} binding sites of the *B. licheniformis* α-amylase with the amino acid sequence SEQ ID NO 2 were determined as described in Example 2 and are as follows:

V102, I103, N104, H105, K106, R125, W155, W157, Y158, H159, F160, D161, G162, T163, Y175, K176, F177, G178, K180, A181, W182, D183, W184, E185, V186, S187, N192, Y193, D194, Y195, L196, M197, Y198, A199, D200, I201, D202, Y203, D204, H205, P206, V208, A209, D231, A232, V233, K234, H235, I236, K237, F238, F240, L241, A294, A295, S296, T297, Q298, G299, G300, G301, Y302, D303, M304, R305, K306, L307, W342, F343, L346, Q393, Y394, Y396, H405, H406, D407, I408, V409, R413, E414, G415, D416, S417, V419, A420, N421, S422, G423, L424, I428, T429, D430, G431, P432, V440, G441, R442, Q443, N444, A445, G446, E447, T448, W449, I462, G475, Y480, V481, Q482, R483.

In order to construct a variant according to this aspect of the invention it is desirable to replace at least one of the above mentioned amino acid residues (or an amino acid residue occupying an equivalent position in another Termamyl-like α-amylase than that defined by SEQ ID NO 2), which is contemplated to be involved in providing a non-optimal calcium binding, with any other amino acid residue which improves the Ca^{2+} binding affinity of the variant enzyme. In practice, the identification and subsequent modification of the amino acid residue is performed by the following method:

i) identifying an amino acid residue within 10Å from a Ca^{2+} binding site of a Termamyl-like α-amylase structure, which from

structural or functional considerations is believed to be responsible for a non-optimal calcium ion interaction,

ii) constructing a variant in which said amino acid residue is replaced with another amino acid residue which from structural or functional considerations is believed to be important for establishing a higher Ca^{2+} binding affinity, and testing the Ca^{2+} dependency of the resulting Termamyl-like α-amylase variant.

In the present context, the term "non-optimal calcium ion interaction" is intended to indicate that the amino acid residue in question is selected on the basis of a presumption that substituting said amino acid residue for another may improve a calcium ion binding interaction of the enzyme. For instance, the amino acid residue in question may be selected on the basis of one or more of the following considerations:

- to obtain an improved interaction between a calcium ion and an amino acid residue located near to the surface of the enzyme (as identified from the structure of the Termamyl-like α-amylase). For instance, if the amino acid residue in question is exposed to a surrounding solvent, it may be advantageous to increase the shielding of said amino acid residue from the solvent so as to provide for a stronger interaction between said amino acid residue and a calcium ion. This can be achieved by replacing said residue (or an amino acid residue in the vicinity of said residue contributing to the shielding) by an amino acid residue which is more bulky or otherwise results in an improved shielding effect.

- to stabilize a calcium binding site, for instance by stabilizing the structure of the Termamyl-like α-amylase (e.g. by stabilizing the contacts between the A, B and C domains or stabilizing one or more of the domains as such). This may, e.g., be achieved by providing for a better coordination to amino acid side chains, which may, e.g., be obtained by replacing an N residue with a D residue and/or a Q residue with

an E residue (e.g. N104D), e.g. within 10Å, and preferably within 3 or 4Å, of a calcium binding site.

- to protect the calcium binding site or to improve the coordination between the calcium ion and the calcium binding site, e.g. by providing a stronger interaction between the ion and the binding site.

Before actually constructing a Termamyl-like α-amylase variant according to the above principles it may be convenient to evaluate the contemplated amino acid modification by its accommodation into the Termamyl-like α-amylase structure, e.g. into a model structure of the parent Termamyl-like α-amylase.

Preferably, the amino acid residue to be modified is located within 8Å of a Ca^{2+} binding site residue, such as within 5Å of such residue. The amino acid residues within 8Å and 5Å, respectively, may easily be identified by an analogous method used for identifying amino acid residues within 10Å (cf. Example 2).

The following mutation is contemplated to be of particular interest with respect to decreasing the Ca^{2+} dependency of a Termamyl-like α-amylase:
N104D (of the *B. licheniformis* α-amylase SEQ ID NO 2, or an equivalent (N to D) mutation of an equivalent position in another Termamyl-like α-amylase.)

In connection with substitutions of relevance for Ca^{2+} dependency, some other substitutions appear to be of importance in stabilizing the enzyme conformation (for instance the Domains A-B and/or Domains A-C interactions contributing to the overall stability of the enzyme) in that they may, e.g., enhance the strength of binding or retention of calcium ion or sodium ion at or within a calcium or sodium binding site, respectively, within the parent Termamyl-like α-amylase.

It is desirable to stabilize the C-domain in order to increase the calcium stability and/or thermostability of the enzyme. In this connection the stabilization may result in a stabilization of the binding of calcium by the enzyme, and an improved contact between the C-domain and the A-domain (of importance for thermostability). The latter may be achieved by introduction of cystein bridges, salt bridges or increase hydrogen, hydrophobic and/or electrostatic interactions.

For instance, the C-domain of the *B. licheniformis* α-amylase having the amino acid sequence shown in SEQ ID No. 2 may be stabilized by introduction of a cystein bridge between domain A and domain C, e.g. by introducing of the following mutations: A349C+I479C and/or L346C+I430C.

A salt bridge may be obtained by introduction of the following mutations:
N457D,E
N457D,E+K385R
F350D,E+I430R,K
F350D,E+I411R,K

The calcium site of Domain C may be stabilized by replacing the amino acid residues H408 and/or G303 with any other amino acid residue. Of particular interest is the following mutations:
H408Q,E,N,D and/or G303N,D,Q,E
which are contemplated to provide a better calcium binding or protection from calcium depletion.

Similar mutations may be introduced in equivalent positions of other Termamyl-like α-amylases.

Other substitution mutations (relative to *B. licheniformis* α-amylase, SEQ ID No. 2) which appear to be of importance, *inter alia*, in the context of reducing calcium dependency include the following: R23K, H156Y, A181T, A209V and G310D (or equivalent mutations in equivalent positions in another Termamyl-like α-amylase). Substitutions of R214 and P345 with

other amino acids may also be of importancen in this connection.

Variants with altered activity at higher/lower pH

It is contemplated that it is possible to change the pH optima of a Termamyl-like α-amylase or the enzymatic activity at a given pH by changing the pKa of the active site residues. This may be achieved, e.g. by changing the electrostatic interaction or hydrophobic interaction between functional groups of amino acid side chains of the amino acid residue to be modified and of its close surroundings. This may, e.g., be accomplished by the following method:

i) in a structure of the Termamyl-like α-amylase in question to identifying an amino acid residue within 15Å from an active site residue, in particulular 10Å from an active site residue, which amino acid residue is contemplated to be involved in electrostatic or hydrophobic interactions with an active site residue,

ii) replacing, in the structure, said amino acid residue with an amino acid residue which changes the electrostatic and/or hydrophobic surroundings of an active site residue and evaluating the accomodation of the amino acid residue in the structure,

iii) optionally repeating step i) and/or ii) until an amino acid replacement has been identified which is accomodated into the structure,

iv) constructing a Termamyl-like α-amylase variant resulting from steps i), ii) and optionally iii) and testing the pH dependent enzymatic activity of interest of said variant.

In the above method it may be of particular relevance to add a positively charged residue within 5Å of a glutamate (thereby lowering the pKa of the glutamate from about 4.5 to 4), or to

add a negatively charged residue within 5 Å of a glutamate (thereby increasing the pKa to about 5), or to make similar modifications within a distance of about 5Å of a Histidine.

In a further aspect the invention relates to a variant of a Termamyl-like α-amylase which exhibits a higher activity at a lower pH (e.g. compared to the pH optimum) than the parent α-amylase. In particular, the variant comprises a mutation of an amino acid residue corresponding to at least one of the following positions of the *B. licheniformis* α-amylase (SEQ ID NO 2):

E336, Q333, P331, I236, V102, A232, I103, L196

The following mutations are of particular interest:

E336R,K
Q333R,K
P331R,K
V102R,K,A,T,S,G;
I236K,R,N;
I103K,R;
L196K,R;
A232T,S,G;

or any combination of two or more of these variants or any combination of one or more of these variants with any of the other variants disclosed herein.

In a still further aspect the invention relates to a variant of a Termamyl-like α-amylase which has a higher activity at a higher pH than the parent α-amylase. In particular, the variant comprises a mutation of an amino acid residue corresponding to at least one of the following positions of the *B. licheniformis* α-amylase (SEQ ID NO 2):

N236, H281, Y273

In particular, the variant comprises a mutation corresponding to at least one of the following mutations of the *B. licheniformis* α-amylase (SEQ ID NO 2):

N326I,Y,F,L,V
H281F,I,L
Y273F,W

or any combination of two or more of these variants or any combination of one or more of these variants with any of the other variants disclosed herein.

A mutation which appears to be importance in relation to the specific activity of variants of the invention is a mutation corresponding to the substitution S187D in *B. licheniformis* α-amylase (SEQ ID NO 2).

<u>Variants with increased thermostability and/or altered temperature optimum</u>

In a further desired aspect the invention relates to a variant of a parent Termamyl-like α-amylase, which variant is the result of one or more amino acid residues having been deleted from, replaced or added to the parent α-amylase so as to obtain an increased thermostability of the variant.

The Termamyl-like α-amylase structure contains a number of unique internal holes, which may contain water, and a number of crevices. In order to increase the thermostability of the α-amylase it may be desirable to reduce the number of holes and crevices (or reduce the size of the holes or crevices), e.g. by introducing one or more hydrophobic contacts, preferably achieved by introducing bulkier residues, in the vicinity or surroundings of the hole. For instance, the amino acid residues to be modified are those which are involved in the formation of the hole.

Accordingly, in a further aspect the present invention relates to a method of increasing the thermostability and/or altering the temperature optimum of a parent Termamyl-like α-amylase, which method comprises

i) identifying an internal hole or a crevice of the parent Termamyl-like α-amylase in the three-dimensional structure of said α-amylase,

ii) replacing, in the structure, one or more amino acid residues in the neighbourhood of the hole or crevice identified in i) with another amino acid residue which from structural or functional considerations is believed to increase the hydrophobic interaction and to fill out or reduce the size of the hole or crevice,

iii) constructing a Termamyl-like α-amylase variant resulting from step ii) and testing the thermostability and/or temperature optimum of the variant.

The structure used for identifying the hole or crevice of the parent Termamyl-like α-amylase may be the structure identified in Appendix 1 or a model structure of the parent Termamyl-like α-amylase built thereon.

It will be understood that the hole or crevice is identified by the amino acid residues surrounding the hole/crevice, and that modification of said amino acid residues are of importance for filling or reducing the size of the hole/crevice. The particular amino acid residues referred to below are those which in crystal structure have been found to flank the hole/crevice in question.

In order to fill (completely or partly) a major hole located between domain A and B, mutation to any other amino acid residue of an amino acid residue corresponding to one or more of the following residues of the *B. licheniformis* α-amylase (SEQ ID NO 2) is contemplated:

L61, Y62, F67, K106, G145, I212, S151, R214, Y150, F143, R146

Of particular interest is a mutation to a more bulky amino acid residue than the amino acid residue of the parent enzyme.

Of particular interest is a variant of a Termamyl-like α-amylase which comprises a mutation corresponding to the following mutations (using the numbering of *B. licheniformis* α-amylase (SEQ ID NO 2):

L61W,V,F;
Y62W;
F67W;
K106R,F,W;
G145F,W
I212F,L,W,Y,R,K;
S151 replaced with any other amino acid residue and in particular with F,W,I or L;
R214W;
Y150R,K;
F143W; and/or
R146W.

In order to fill a hole in the vicinity of the active site mutation to any other amino acid residue of an amino acid residue corresponding to one or more of the following residues of the *B. licheniformis* α-amylase (SEQ ID NO 2) is contemplated:

L241, I236.

Of interest is a mutation to a more bulky amino acid residue.

Of particular interest is a variant of a Termamyl-like α-amylase which comprises a mutation corresponding to one or more of the following mutations in the *B. licheniformis* α-amylase:

L241I,F,Y,W; and/or
I236L,F,W,Y

In order to fill a hole in the vicinity of the active site mutation to any other amino acid residue of an amino acid residue corresponding to one or more of the following residues of the *B. licheniformis* α-amylase (SEQ ID NO 2) is contemplated:
L7, V259, F284

Of interest is a mutation to a more bulky amino acid residue.

Of particular interest is a variant of a Termamyl-like α-amylase which comprises a mutation corresponding to one or more of the following mutations in the *B. licheniformis* α-amylase:

L7F,I,W
V259F,I,L
F284W

In order to fill a hole in the vicinity of the active site mutation to any other amino acid residue of an amino acid residue corresponding to one or more of the following residues of the *B. licheniformis* α-amylase (SEQ ID NO 2) is contemplated:

F350, F343

Of interest is a mutation to a more bulky amino acid residue.

Of particular interest is a variant of a Termamyl-like α-amylase which comprises a mutation corresponding to one or more of the following mutations in the *B. licheniformis* α-amylase:
F350W

F343W

In order to fill a hole in the vicinity of the active site mutation to any other amino acid residue of an amino acid residue corresponding to one or more of the following residues of the *B. licheniformis* α-amylase (SEQ ID NO 2) is contemplated:

L427, V481

Of interest is a mutation to a more bulky amino acid residue.

Of particular interest is a variant of a Termamyl-like α-amylase which comprises a mutation corresponding to one or more of the following mutations in the *B. licheniformis* α-amylase:

L427F,L,W
V481,F,I,L,W

<u>Variants with an altered cleavage pattern</u>
In the starch liquefaction process it is desirable to use an α-amylase which is capable of degrading the starch molecules into long branched oligo saccharides (like, e.g. the Fungamyl-like α-amylases) rather than shorter branched oligo saccharides (like conventional Termamyl-like α-amylases). The resulting very small branched oligosaccharides (panose precursors) cannot be hydrolyzed properly by pullulanases, which in the liquefaction process are used after the α-amylases and before the amyloglucosidases. Thus, in the presence of panose precursors the action of amylo-glucoamylase ends up with a high degree of the small branched limiting-dextrin, the trisaccharide panose. The presence of panose lowers the saccharification yield significantly and is thus undesirable.

Thus, one aim of the present invention is to change the degradation characteristics of a Termamyl-like α-amylase to that of a Fungamyl-like α-amylases without at the same time reducing the thermostability of the Termamyl-like α-amylase.

Accordingly, in a further aspect the invention relates to a variant of a Termamyl-like α-amylase which has a reduced ability to cleave a substrate close to the branching point.

The variant may suitably be constructed by a method which comprises

i) identifying the substrate binding area of the parent Termamyl-like α-amylase in a model of the three-dimensional structure of said α-amylase, (e.g. within a sphere of 4Å from the substrate binding site (as defined in the section above entitled "Substrate Binding Site"),

ii) replacing, in the model, one or more amino acid residues of the substrate binding area of the cleft identified in i), which is/are believed to be responsible for the cleavage pattern of the parent α-amylase, with another amino acid residue which from structural considerations is believed to result in an altered substrate cleavage pattern, or deleting one or more amino acid residues of the substrate binding area contemplated to introduce favourable interactions to the substrate or adding one or more amino acid residues to the substrate binding area contemplated to introduce favourable interactions to the substrate, and

iii) constructing a Termamyl-like α-amylase variant resulting from step ii) and testing the substrate cleavage pattern of the variant.

Of particular interest is a variant which cleaves an amylopectin substrate, from the reducing end, more than one glucose unit from the branching point, preferably more than two or three glucose units from the branching point, i.e. at a further distance from the branching point than that obtained by use of a wild type *B. licheniformis* α-amylase.

Residues of particular interest in connection with this aspect of the invention correspond to the following residues of the *B. licheniformis* α-amylase (SEQ ID NO 2): V54, D53, Y56, Q333,

G57, and the variants according to this aspect preferably comprises a mutation in one or more of these residues.

In particular, the variant comprises at least one of the following mutations, which are expected to prevent cleavage close to the branching point:

V54L,I,F,Y,W,R,K,H,E,Q
D53L,I,F,Y,W
Y56W
Q333W
G57all possible amino acid residues
A52amino acid residues larger than A, e.g. A52W,Y,L,F,I.

<u>Variants of a fungal α-amylase</u>

In a still further embodiment the invention relates to a variant of a parent Fungamyl-like α-amylase, in which variant at least one of the amino acid residues of the parent α-amylase, which is/are present in an amino acid fragment corresponding to amino acid residues 291-313 of the amino acid sequence of SEQ ID No. 10, has/have been deleted or replaced with one or more of the amino acid residues, which is/are present in an amino acid fragment corresponding to amino acid residues 98-210 of the amino acid sequence shown in SEQ ID No. 4, or in which one or more additional amino acid residues has/have been inserted using the relevant part of SEQ ID No. 4 or a corresponding part of another Termamyl-like α-amylase as a template.

For instance, the variant may be one, in which the amino acid fragment X-Y of the parent α-amylase, which corresponds to or is within the amino acid fragment 117-185 of SEQ ID No. 10, has/have been replaced with an amino acid fragment Z-V, which corresponds to or is within the amino acid fragment 98-210 of the amino acid sequence shown in SEQ ID No. 4, in which variant

X is an amino acid residue corresponding to the amino acid occupying position 117, 118, 119, 120 or 121 of SEQ ID No. 10,

Y is an amino acid residue corresponding to the amino acid occupying position 181, 182, 183, 184 or 185 of SEQ ID No. 10,

Z is an amino acid residue corresponding to the amino acid occupying position 98, 99, 100, 101 or 102 of SEQ ID No. 4, and

V is an amino acid residue corresponding to the amino acid occupying position 206, 207, 208, 209 or 210 of SEQ ID No. 4.

A specific example of a variant according to this aspect of the invention is one, in which the amino acid fragment of the parent α-amylase, which corresponds to amino acid residues 121-181 of SEQ ID No. 10, has been replaced with the amino acid fragment corresponding to amino acid residues 102-206 of the amino acid sequence shown in SEQ ID No. 4.

Another example of a variant according to this aspect of the invention is one, in which the amino acid fragment of the parent α-amylase, which corresponds to amino acid residues 121-174 of SEQ ID No. 10, has been replaced with the amino acid fragment corresponding to amino acid residues 102-199 of the amino acid sequence shown in SEQ ID No. 4.

In a further embodiment the invention relates to a variant of a parent Fungamyl-like α-amylase, in which an amino acid fragment corresponding to amino acid residues 181-184 of the amino acid sequence shown in SEQ ID No. 10 has been deleted.

General mutations in variants of the invention

It may be preferred that the variant of the invention or prepared in accordance with the method of the invention comprises one or more modifications in addition to those outlined above. Thus, it may be advantageous that one or more proline residues present in the part of the α-amylase variant

having been modified is/are replaced with a non-proline residue which may be any of the possible, naturally occurring non-proline residues, and which preferably is an alanine, glycine, serine, threonine, valine or leucine.

Analogously, it may be preferred that one or more cysteine residues present in the amino acid residues with which the parent α-amylase is modified are replaced with a non-cysteine residues such as serine, alanine, threonine, glycine, valine or leucine.

Furthermore, the variant of the invention may either as the only modification or in combination with any of the above outlined modifications be modified so that one or more Asp and/or Glu present in an amino acid fragment corresponding to the amino acid fragment 185-209 of SEQ ID No. 8 is replaced by an Asn and/or Gln, respectively. Also of interest is the modification of one or more of the Lys residues present in the Termamyl-like α-amylase is replaced by an Arg present in an amino acid fragment corresponding to the amino acid fragment 185-209 of SEQ ID No. 8 is replaced by an Asn and/or Gln, respectively.

It will be understood that in accordance with the present invention variants may be prepared which carry two or more of the above outlined modifications. For instance, variants may be prepared which comprises a modification in the loop 1 and loop 2 region, a modification in loop 2 and limited loop 3, a modification in loop 1, loop 2, loop 3 and loop 8, etc.

Furthermore, it may be advantageous to introduce point-mutations in any of the variants described herein.

<u>Methods of preparing α-amylase variants</u>

Several methods for introducing mutations into genes are known in the art. After a brief discussion of the cloning of α-amylase-encoding DNA sequences, methods for generating

mutations at specific sites within the α-amylase-encoding sequence will be discussed.

Cloning a DNA sequence encoding an α-amylase

The DNA sequence encoding a parent α-amylase may be isolated from any cell or microorganism producing the α-amylase in question, using various methods well known in the art. First, a genomic DNA and/or cDNA library should be constructed using chromosomal DNA or messenger RNA from the organism that produces the α-amylase to be studied. Then, if the amino acid sequence of the α-amylase is known, homologous, labelled oligonucleotide probes may be synthesized and used to identify α-amylase-encoding clones from a genomic library prepared from the organism in question. Alternatively, a labelled oligonucleotide probe containing sequences homologous to a known α-amylase gene could be used as a probe to identify α-amylase-encoding clones, using hybridization and washing conditions of lower stringency.

Yet another method for identifying α-amylase-encoding clones would involve inserting fragments of genomic DNA into an expression vector, such as a plasmid, transforming α-amylase-negative bacteria with the resulting genomic DNA library, and then plating the transformed bacteria onto agar containing a substrate for α-amylase, thereby allowing clones expressing the α-amylase to be identified.

Alternatively, the DNA sequence encoding the enzyme may be prepared synthetically by established standard methods, e.g. the phosphoroamidite method described by S.L. Beaucage and M.H. Caruthers (1981) or the method described by Matthes et al. (1984). In the phosphoroamidite method, oligonucleotides are synthesized, e.g. in an automatic DNA synthesizer, purified, annealed, ligated and cloned in appropriate vectors.

Finally, the DNA sequence may be of mixed genomic and synthetic origin, mixed synthetic and cDNA origin or mixed genomic and cDNA origin, prepared by ligating fragments of synthetic,

genomic or cDNA origin (as appropriate, the fragments corresponding to various parts of the entire DNA sequence), in accordance with standard techniques. The DNA sequence may also be prepared by polymerase chain reaction (PCR) using specific primers, for instance as described in US 4,683,202 or R.K. Saiki et al. (1988).

Site-directed mutagenesis

Once an α-amylase-encoding DNA sequence has been isolated, and desirable sites for mutation identified, mutations may be introduced using synthetic oligonucleotides. These oligonucleotides contain nucleotide sequences flanking the desired mutation sites; mutant nucleotides are inserted during oligonucleotide synthesis. In a specific method, a single-stranded gap of DNA, bridging the α-amylase-encoding sequence, is created in a vector carrying the α-amylase gene. Then the synthetic nucleotide, bearing the desired mutation, is annealed to a homologous portion of the single-stranded DNA. The remaining gap is then filled in with DNA polymerase I (Klenow fragment) and the construct is ligated using T4 ligase. A specific example of this method is described in Morinaga et al. (1984). US 4,760,025 discloses the introduction of oligonucleotides encoding multiple mutations by performing minor alterations of the cassette. However, an even greater variety of mutations can be introduced at any one time by the Morinaga method, because a multitude of oligonucleotides, of various lengths, can be introduced.

Another method of introducing mutations into α-amylase-encoding DNA sequences is described in Nelson and Long (1989). It involves the 3-step generation of a PCR fragment containing the desired mutation introduced by using a chemically synthesized DNA strand as one of the primers in the PCR reactions. From the PCR-generated fragment, a DNA fragment carrying the mutation may be isolated by cleavage with restriction endonucleases and reinserted into an expression plasmid.

Random mutagenesis

Random mutagenesis is suitably performed either as localized or region-specific random mutagenesis in at least three parts of the gene translating to the amino acid sequence shown in question, or within the whole gene.

For region-specific random mutagenesis with a view to improving the thermal stability of a parent Termamyl-like α-amylase, codon positions corresponding to the following amino acid residues of the *B. licheniformis* α-amylase (SEQ ID NO 2) may appropriately be targeted:

<u>To improve the stability of the calcium site between Domain A and C</u>

I428-A435
T297-L308
F403-V409

<u>To improve the stability between domain A and B:</u>

D180-D204
H156-T163
A232-F238

With a view to achieving improved binding of a substrate (i.e. improved binding of a carbohydrate species, such as amylose or amylopectin) by a Termamyl-like α-amylase variant, modified (e.g. higher) substrate specificity and/or modified (e.g. higher) specificity with respect to cleavage (hydrolysis) of substrate, it appears that the following codon positions for the amino acid sequence shown in SEQ ID NO 2 (or equivalent codon positions for another parent Termamyl-like α-amylase in the context of the invention) may particularly appropriately be targeted:

13-18
50-56
70-76
102-109
163-172

189-199
229-235
360-264
327-335

The random mutagenesis of a DNA sequence encoding a parent α-amylase to be performed in accordance with step a) of the above-described method of the invention may conveniently be performed by use of any method known in the art.

For instance, the random mutagenesis may be performed by use of a suitable physical or chemical mutagenizing agent, by use of a suitable oligonucleotide, or by subjecting the DNA sequence to PCR generated mutagenesis. Furthermore, the random mutagenesis may be performed by use of any combination of these mutagenizing agents.

The mutagenizing agent may, e.g., be one which induces transitions, transversions, inversions, scrambling, deletions, and/or insertions.

Examples of a physical or chemical mutagenizing agent suitable for the present purpose include ultraviolet (UV) irradiation, hydroxylamine, N-methyl-N'-nitro-N-nitrosoguanidine (MNNG), O-methyl hydroxylamine, nitrous acid, ethyl methane sulphonate (EMS), sodium bisulphite, formic acid, and nucleotide analogues.

When such agents are used, the mutagenesis is typically performed by incubating the DNA sequence encoding the parent enzyme to be mutagenized in the presence of the mutagenizing agent of choice under suitable conditions for the mutagenesis to take place, and selecting for mutated DNA having the desired properties.

When the mutagenesis is performed by the use of an oligonucleotide, the oligonucleotide may be doped or spiked with the three non-parent nucleotides during the synthesis of the oligonucleo-

tide at the positions which are to be changed. The doping or spiking may be done so that codons for unwanted amino acids are avoided. The doped or spiked oligonucleotide can be incorporated into the DNA encoding the amylolytic enzyme by any published technique, using e.g. PCR, LCR or any DNA polymerase and ligase.

When PCR-generated mutagenesis is used, either a chemically treated or non-treated gene encoding a parent α-amylase enzyme is subjected to PCR under conditions that increase the mis-incorporation of nucleotides (Deshler 1992; Leung et al., Technique, Vol.1, 1989, pp. 11-15).

A mutator strain of *E. coli* (Fowler et al., Molec. Gen. Genet., 133, 1974, pp. 179-191), *S. cereviseae* or any other microbial organism may be used for the random mutagenesis of the DNA encoding the amylolytic enzyme by e.g. transforming a plasmid containing the parent enzyme into the mutator strain, growing the mutator strain with the plasmid and isolating the mutated plasmid from the mutator strain. The mutated plasmid may subsequently be transformed into the expression organism.

The DNA sequence to be mutagenized may conveniently be present in a genomic or cDNA library prepared from an organism expressing the parent amylolytic enzyme. Alternatively, the DNA sequence may be present on a suitable vector such as a plasmid or a bacteriophage, which as such may be incubated with or otherwise exposed to the mutagenizing agent. The DNA to be mutagenized may also be present in a host cell either by being integrated in the genome of said cell or by being present on a vector harboured in the cell. Finally, the DNA to be mutagenized may be in isolated form. It will be understood that the DNA sequence to be subjected to random mutagenesis is preferably a cDNA or a genomic DNA sequence.

In some cases it may be convenient to amplify the mutated DNA sequence prior to the expression step (b) or the screening step (c) being performed. Such amplification may be performed in

accordance with methods known in the art, the presently preferred method being PCR-generated amplification using oligonucleotide primers prepared on the basis of the DNA or amino acid sequence of the parent enzyme.

Subsequent to the incubation with or exposure to the mutagenizing agent, the mutated DNA is expressed by culturing a suitable host cell carrying the DNA sequence under conditions allowing expression to take place. The host cell used for this purpose may be one which has been transformed with the mutated DNA sequence, optionally present on a vector, or one which was carried the DNA sequence encoding the parent enzyme during the mutagenesis treatment. Examples of suitable host cells are the following: grampositive bacteria such as *Bacillus subtilis*, *Bacillus licheniformis*, *Bacillus lentus*, *Bacillus brevis*, *Bacillus stearothermophilus*, *Bacillus alkalophilus*, *Bacillus amyloliquefaciens*, *Bacillus coagulans*, *Bacillus circulans*, *Bacillus lautus*, *Bacillus megaterium*, *Bacillus thuringiensis*, *Streptomyces lividans* or *Streptomyces murinus*; and gramnegative bacteria such as *E.coli*.

The mutated DNA sequence may further comprise a DNA sequence encoding functions permitting expression of the mutated DNA sequence.

Localized random mutagenesis: the random mutagenesis may advantageously be localized to a part of the parent α-amylase in question. This may, e.g., be advantageous when certain regions of the enzyme have been identified to be of particular importance for a given property of the enzyme, and when modified are expected to result in a variant having improved properties. Such regions may normally be identified when the tertiary structure of the parent enzyme has been elucidated and related to the function of the enzyme.

The localized random mutagenesis is conveniently performed by use of PCR- generated mutagenesis techniques as described above or any other suitable technique known in the art.

Alternatively, the DNA sequence encoding the part of the DNA sequence to be modified may be isolated, e.g. by being inserted into a suitable vector, and said part may subsequently be subjected to mutagenesis by use of any of the mutagenesis methods discussed above.

With respect to the screening step in the above-mentioned method of the invention, this may conveniently performed by use of aa filter assay based on the following principle:

A microorganism capable of expressing the mutated amylolytic enzyme of interest is incubated on a suitable medium and under suitable conditions for the enzyme to be secreted, the medium being provided with a double filter comprising a first protein-binding filter and on top of that a second filter exhibiting a low protein binding capability. The microorganism is located on the second filter. Subsequent to the incubation, the first filter comprising enzymes secreted from the microorganisms is separated from the second filter comprising the microorganisms. The first filter is subjected to screening for the desired enzymatic activity and the corresponding microbial colonies present on the second filter are identified.

The filter used for binding the enzymatic activity may be any protein binding filter e.g. nylon or nitrocellulose. The top-filter carrying the colonies of the expression organism may be any filter that has no or low affinity for binding proteins e.g. cellulose acetate or Durapore™. The filter may be pretreated with any of the conditions to be used for screening or may be treated during the detection of enzymatic activity.

The enzymatic activity may be detected by a dye, fluorescence, precipitation, pH indicator, IR-absorbance or any other known technique for detection of enzymatic activity.

The detecting compound may be immobilized by any immobilizing agent e.g. agarose, agar, gelatine, polyacrylamide, starch, filter paper, cloth; or any combination of immobilizing agents.

α-Amylase activity is detected by Cibacron Red labelled amylopectin, which is immobilized on agarose. For screening for variants with increased thermal and high-pH stability, the filter with bound α-amylase variants is incubated in a buffer at pH 10.5 and 60° or 65°C for a specified time, rinsed briefly in deionized water and placed on the amylopectin-agarose matrix for activity detection. Residual activity is seen as lysis of Cibacron Red by amylopectin degradation. The conditions are chosen to be such that activity due to the α-amylase having the amino acid sequence shown in SEQ ID No.1 can barely be detected. Stabilized variants show, under the same conditions, increased colour intensity due to increased liberation of Cibacron Red.

For screening for variants with an activity optimum at a lower temperature and/or over a broader temperature range, the filter with bound variants is placed directly on the amylopectin-Cibacron Red substrate plate and incubated at the desired temperature (e.g. 4°C, 10°C or 30°C) for a specified time. After this time activity due to the α-amylase having the amino acid sequence shown in SEQ ID No.1 can barely be detected, whereas variants with optimum activity at a lower temperature will show increase amylopectin lysis. Prior to incubation onto the amylopectin matrix, incubation in all kinds of desired media - e.g. solutions containing Ca^{2+}, detergents, EDTA or other relevant additives - can be carried out in order to screen for changed dependency or for reaction of the variants in question with such additives.

Testing of variants of the invention

The testing of variants of the invention may suitably be performed by determining the starch-degrading activity of the variant, for instance by growing host cells transformed with a DNA sequence encoding a variant on a starch-containing agarose plate and identifying starch-degrading host cells. Further testing as to altered properties (including specific activity,

substrate specificity, cleavage pattern, thermoactivation, pH optimum, pH dependency, temperature optimum, and any other parameter) may be performed in accordance with methods known in the art.

Expression of α-amylase variants

According to the invention, a DNA sequence encoding the variant produced by methods described above, or by any alternative methods known in the art, can be expressed, in enzyme form, using an expression vector which typically includes control sequences encoding a promoter, operator, ribosome binding site, translation initiation signal, and, optionally, a repressor gene or various activator genes.

The recombinant expression vector carrying the DNA sequence encoding an α-amylase variant of the invention may be any vector which may conveniently be subjected to recombinant DNA procedures, and the choice of vector will often depend on the host cell into which it is to be introduced. Thus, the vector may be an autonomously replicating vector, i.e. a vector which exists as an extrachromosomal entity, the replication of which is independent of chromosomal replication, e.g. a plasmid, a bacteriophage or an extrachromosomal element, minichromosome or an artificial chromosome. Alternatively, the vector may be one which, when introduced into a host cell, is integrated into the host cell genome and replicated together with the chromosome(s) into which it has been integrated.

In the vector, the DNA sequence should be operably connected to a suitable promoter sequence. The promoter may be any DNA sequence which shows transcriptional activity in the host cell of choice and may be derived from genes encoding proteins either homologous or heterologous to the host cell. Examples of suitable promoters for directing the transcription of the DNA sequence encoding an α-amylase variant of the invention, especially in a bacterial host, are the promoter of the *lac* operon of *E.coli*, the *Streptomyces coelicolor* agarase gene *dag*A promoters, the promoters of the *Bacillus licheniformis* α-

amylase gene (*amyL*), the promoters of the *Bacillus stearothermophilus* maltogenic amylase gene (*amyM*), the promoters of the *Bacillus amyloliquefaciens* α-amylase (*amyQ*), the promoters of the *Bacillus subtilis* xylA and xylB genes etc. For transcription in a fungal host, examples of useful promoters are those derived from the gene encoding *A. oryzae* TAKA amylase, *Rhizomucor miehei* aspartic proteinase, *A. niger* neutral α-amylase, *A. niger* acid stable α-amylase, *A. niger* glucoamylase, *Rhizomucor miehei* lipase, *A. oryzae* alkaline protease, *A. oryzae* triose phosphate isomerase or *A. nidulans* acetamidase.

The expression vector of the invention may also comprise a suitable transcription terminator and, in eukaryotes, polyadenylation sequences operably connected to the DNA sequence encoding the α-amylase variant of the invention. Termination and polyadenylation sequences may suitably be derived from the same sources as the promoter.

The vector may further comprise a DNA sequence enabling the vector to replicate in the host cell in question. Examples of such sequences are the origins of replication of plasmids pUC19, pACYC177, pUB110, pE194, pAMB1 and pIJ702.

The vector may also comprise a selectable marker, e.g. a gene the product of which complements a defect in the host cell, such as the *dal* genes from *B. subtilis* or *B. licheniformis*, or one which confers antibiotic resistance such as ampicillin, kanamycin, chloramphenicol or tetracyclin resistance. Furthermore, the vector may comprise *Aspergillus* selection markers such as amdS, argB, niaD and sC, a marker giving rise to hygromycin resistance, or the selection may be accomplished by co-transformation, e.g. as described in WO 91/17243.

While intracellular expression may be advantageous in some respects, e.g. when using certain bacteria as host cells, it is generally preferred that the expression is extracellular. In general, the *Bacillus* α-amylases mentioned herein comprise a

preregion permitting secretion of the expressed protease into the culture medium. If desirable, this preregion may be replaced by a different preregion or signal sequence, conveniently accomplished by substitution of the DNA sequences encoding the respective preregions.

The procedures used to ligate the DNA construct of the invention encoding an α-amylase variant, the promoter, terminator and other elements, respectively, and to insert them into suitable vectors containing the information necessary for replication, are well known to persons skilled in the art (cf., for instance, Sambrook et al. (1989)).

The cell of the invention, either comprising a DNA construct or an expression vector of the invention as defined above, is advantageously used as a host cell in the recombinant production of an α-amylase variant of the invention. The cell may be transformed with the DNA construct of the invention encoding the variant, conveniently by integrating the DNA construct (in one or more copies) in the host chromosome. This integration is generally considered to be an advantage as the DNA sequence is more likely to be stably maintained in the cell. Integration of the DNA constructs into the host chromosome may be performed according to conventional methods, e.g. by homologous or heterologous recombination. Alternatively, the cell may be transformed with an expression vector as described above in connection with the different types of host cells.

The cell of the invention may be a cell of a higher organism such as a mammal or an insect, but is preferably a microbial cell, e.g. a bacterial or a fungal (including yeast) cell.

Examples of suitable bacteria are grampositive bacteria such as *Bacillus subtilis*, *Bacillus licheniformis*, *Bacillus lentus*, *Bacillus brevis*, *Bacillus stearothermophilus*, *Bacillus alkalophilus*, *Bacillus amyloliquefaciens*, *Bacillus coagulans*, *Bacillus circulans*, *Bacillus lautus*, *Bacillus megaterium*, *Bacillus thuringiensis*, or *Streptomyces lividans* or *Streptomyces*

murinus, or gramnegative bacteria such as *E.coli*. The transformation of the bacteria may, for instance, be effected by protoplast transformation or by using competent cells in a manner known *per se*.

The yeast organism may favourably be selected from a species of *Saccharomyces* or *Schizosaccharomyces*, e.g. *Saccharomyces cerevisiae*. The filamentous fungus may advantageously belong to a species of *Aspergillus*, e.g. *Aspergillus oryzae* or *Aspergillus niger*. Fungal cells may be transformed by a process involving protoplast formation and transformation of the protoplasts followed by regeneration of the cell wall in a manner known *per se*. A suitable procedure for transformation of *Aspergillus* host cells is described in EP 238 023.

In a yet further aspect, the present invention relates to a method of producing an α-amylase variant of the invention, which method comprises cultivating a host cell as described above under conditions conducive to the production of the variant and recovering the variant from the cells and/or culture medium.

The medium used to cultivate the cells may be any conventional medium suitable for growing the host cell in question and obtaining expression of the α-amylase variant of the invention. Suitable media are available from commercial suppliers or may be prepared according to published recipes (e.g. as described in catalogues of the American Type Culture Collection).

The α-amylase variant secreted from the host cells may conveniently be recovered from the culture medium by well-known procedures, including separating the cells from the medium by centrifugation or filtration, and precipitating proteinaceous components of the medium by means of a salt such as ammonium sulphate, followed by the use of chromatographic procedures such as ion exchange chromatography, affinity chromatography, or the like.

Industrial Applications

The α-amylase variants of this invention possesses valuable properties allowing for various industrial applications. In particular the enzyme variants finds potential applications as a component in washing, dishwashing and hard surface cleaning detergent compositions, but it may also be useful in the production of sweeteners and ethanol from starch and for textile desizing. Conditions for conventional starch converting processes and liquefaction and/or saccharification processes are described in for instance US Patent No. 3,912,590 and EP patent publications Nos. 252,730 and 63,909.

Production of sweetners from starch: A "traditional" process for conversion of starch to fructose syrups normally consists of three consecutive enzymatic processes, viz. a liquefaction process followed by a saccharification process and an isomerization process. During the liquefaction process, starch is degraded to dextrins by an α-amylase (e.g. Termamyl™) at pH values between 5.5 and 6.2 and at temperatures of 95-160°C for a period of approx. 2h. In order to ensure an optimal enzyme stability under these conditions, 1mM of calcium is added (40 ppm free calcium ions).

After the liquefaction process the dextrins are converted into dextrose by addition of a glucoamylase (e.g. AMG™) and a debranching enzyme, such as an isoamylase or a pullulanase (e.g. Promozyme™). Before this step the pH is reduced to a value below 4.5, maintaining the high temperature (above 95°C), and the liquefying α-amylase activity is denatured. The temperature is lowered to 60°C, and glucoamylase and debranching enzyme are added. The saccharification process proceeds for 24-72 hours.

After the saccharification process the pH is increased to a value in the range of 6-8, preferably pH 7.5, and the calcium is removed by ion exchange. The dextrose syrup is then converted into high fructose syrup using, e.g., an immmobilized glucoseisomerase (such as Sweetzyme™).

At least 3 enzymatic improvements of this process could be obtained. All three improvements could be seen as individual benefits, but any combination (e.g. 1+2, 1+3, 2+3 or 1+2+3) could be employed:

Improvement 1. Reduction of the calcium dependency of the liquefying alpha-amylase.

Addition of free calcium is required to ensure adequately high stability of the α-amylase, but free calcium strongly inhibits the activity of the glucoseisomerase and needs to be removed, by means of an expensive unit operation, to an extent which reduces the level of free calcium to below 3-5 ppm. Cost savings could be obtained if such an operation could be avoided and the liquefaction process could be performed without addition of free calcium ions.

To achieve that, a less calcium-dependent Termamyl-like α-amylase which is stable and highly active at low concentrations of free calcium (< 40 ppm) is required. Such a Termamyl-like α-amylase should have a pH optimum at a pH in the range of 4.5-6.5, preferably in the range of 4.5-5.5.

Improvement 2. Reduction of formation of unwanted Maillard products

The extent of formation of unwanted Maillard products during the liquefaction process is dependent on the pH. Low pH favours reduced formation of Maillard products. It would thus be desirable to be able to lower the process pH from around pH 6.0 to a value around pH 4.5; unfortunately, all commonly known, thermostable Termamyl-like α-amylases are not very stable at low pH (i.e. pH < 6.0) and their specific activity is generally low.

Achievement of the above-mentioned goal requires a Termamyl-like α-amylase which is stable at low pH in the range of

4.5-5.5 and at free calcium concentrations in the range of 0-40 ppm, and which maintains a high specific activity.

Improvement 3.

It has been reported previously (US patent 5,234,823) that when saccharifying with *A. niger* glucoamylase and *B. acidopullulyticus* pullulanase, the presence of residual α-amylase activity from the liquefaction process can lead to lower yields of dextrose if the α-amylase is not inactivated before the saccharification stage. This inactivation can typically be carried out by adjusting the pH to below 4.3 at 95°C, before lowering the temperature to 60°C for saccharification.

The reason for this negative effect on dextrose yield is not fully understood, but it is assumed that the liquefying α-amylase (for example Termamyl™ 120 L from *B. licheniformis*) generates "limit dextrins" (which are poor substrates for *B. acidopullulyticus* pullulanase) by hydrolysing 1,4-alpha-glucosidic linkages close to and on both sides of the branching points in amylopectin. Hydrolysis of these limit dextrins by glucoamylase leads to a build-up of the trisaccharide panose, which is only slowly hydrolysed by glucoamylase.

The development of a thermostable α-amylase which does not suffer from this disadvantage would be a significant process improvement, as no separate inactivation step would be required.

If a Termamyl-like, low-pH-stable α-amylase is developed, an alteration of the specificity could be an advantage needed in combination with increased stability at low pH.

The methodology and principles of the present invention make it possible to design and produce variants according to the invention having the required properties as outlined above.

Detergent Compositions

According to the invention, the α-amylase may typically be a component of a detergent composition. As such, it may be included in the detergent composition in the form of a non-dusting granulate, a stabilized liquid, or a protected enzyme. Non-dusting granulates may be produced, e.g. as disclosed in US 4,106,991 and 4,661,452 (both to Novo Industri A/S) and may optionally be coated by methods known in the art. Examples of waxy coating materials are poly(ethylene oxide) products (polyethyleneglycol, PEG) with mean molar weights of 1000 to 20000, ethoxylated nonylphenols having from 16 to 50 ethylene oxide units; ethoxylated fatty alcohols in which the alcohol contains from 12 to 20 carbon atoms and in which there are 15 to 80 ethylene oxide units; fatty alcohols; fatty acids; and mono- and di- and triglycerides of fatty acids. Examples of film-forming coating materials suitable for application by fluid bed techniques are given in patent GB 1483591. Liquid enzyme preparations may, for instance, be stabilized by adding a polyol such as propylene glycol, a sugar or sugar alcohol, lactic acid or boric acid according to established methods. Other enzyme stabilizers are well known in the art. Protected enzymes may be prepared according to the method disclosed in EP 238,216.
The detergent composition of the invention may be in any convenient form, e.g. as powder, granules, paste or liquid. A liquid detergent may be aqueous, typically containing up to 70% of water and 0-30% of organic solvent, or nonaqueous.

The detergent composition comprises one or more surfactants, each of which may be anionic, nonionic, cationic, or zwitter-ionic. The detergent will usually contain 0-50% of anionic surfactant such as linear alkylbenzenesulfonate (LAS), alpha-olefinsulfonate (AOS), alkyl sulfate (fatty alcohol sulfate) (AS), alcohol ethoxysulfate (AEOS or AES), secondary alkane-sulfonates (SAS), alpha-sulfo fatty acid methyl esters, alkyl- or alkenylsuccinic acid or soap. It may also contain 0-40% of nonionic surfactant such as alcohol ethoxylate (AEO or AE), carboxylated alcohol ethoxylates, nonylphenol ethoxylate, alkylpolyglycoside, alkyldimethylamineoxide, ethoxylated fatty

acid monoethanolamide, fatty acid monoethanolamide, or polyhydroxy alkyl fatty acid amide (e.g. as described in WO 92/06154).

The detergent composition may additionally comprise one or more other enzymes, such as lipase, cutinase, protease, cellulase, peroxidase, e.g., laccase.

The detergent may contain 1-65% of a detergent builder or complexing agent such as zeolite, diphosphate, triphosphate, phosphonate, citrate, nitrilotriacetic acid (NTA), ethylenediaminetetraacetic acid (EDTA), diethylenetriaminepentaacetic acid (DTMPA), alkyl- or alkenylsuccinic acid, soluble silicates or layered silicates (e.g. SKS-6 from Hoechst). The detergent may also be unbuilt, i.e. essentially free of detergent builder.

The detergent may comprise one or more polymers. Examples are carboxymethylcellulose (CMC), poly(vinylpyrrolidone) (PVP), polyethyleneglycol (PEG), poly(vinyl alcohol) (PVA), polycarboxylates such as polyacrylates, maleic/acrylic acid copolymers and lauryl methacrylate/acrylic acid copolymers.

The detergent may contain a bleaching system which may comprise a H_2O_2 source such as perborate or percarbonate which may be combined with a peracid-forming bleach activator such as tetraacetylethylenediamine (TAED) or nonanoyloxybenzenesulfonate (NOBS). Alternatively, the bleaching system may comprise peroxy acids of e.g. the amide, imide, or sulfone type.

The enzymes of the detergent composition of the invention may be stabilized using conventional stabilizing agents, e.g. a polyol such as propylene glycol or glycerol, a sugar or sugar alcohol, lactic acid, boric acid, or a boric acid derivative as e.g. an aromatic borate ester, and the composition may be formulated as described in e.g. WO 92/19709 and WO 92/19708.

The detergent may also contain other conventional detergent ingredients such as e.g. fabric conditioners including clays, foam boosters, suds suppressors, anti-corrosion agents, soil-suspending agents, anti-soil redeposition agents, dyes, bactericides, optical brighteners, or perfume.

The pH (measured in aqueous solution at use concentration) will usually be neutral or alkaline, e.g. 7-11.

Particular forms of detergent compositions within the scope of the invention include:

1) A detergent composition formulated as a granulate having a bulk density of at least 600 g/l comprising

Linear alkylbenzenesulfonate (calculated as acid)	7 - 12%
Alcohol ethoxysulfate (e.g. C_{12-18} alcohol, 1-2 EO) or alkyl sulfate (e.g. C_{16-18})	1 - 4%
Alcohol ethoxylate (e.g. C_{14-15} alcohol, 7 EO)	5 - 9%
Sodium carbonate (as Na_2CO_3)	14 - 20%
Soluble silicate (as $Na_2O,2SiO_2$)	2 - 6%
Zeolite (as $NaAlSiO_4$)	15 - 22%
Sodium sulfate (as Na_2SO_4)	0 - 6%
Sodium citrate/citric acid (as $C_6H_5Na_3O_7/C_6H_8O_7$)	0 - 15%
Sodium perborate (as $NaBO_3.H_2O$)	11 - 18%
TAED	2 - 6%
Carboxymethylcellulose	0 - 2%
Polymers (e.g. maleic/acrylic acid copolymer, PVP, PEG)	0 - 3%
Enzymes (calculated as pure enzyme protein)	0.0001 - 0.1%
Minor ingredients (e.g. suds suppressors, perfume, optical brightener, photobleach)	0 - 5%

2) A detergent composition formulated as a granulate having a bulk density of at least 600 g/l comprising

Linear alkylbenzenesulfonate (calculated as acid)	6 - 11%
Alcohol ethoxysulfate (e.g. C_{12-18} alcohol, 1-2 EO or alkyl sulfate (e.g. C_{16-18})	1 - 3%
Alcohol ethoxylate (e.g. C_{14-15} alcohol, 7 EO)	5 - 9%
Sodium carbonate (as Na_2CO_3)	15 - 21%
Soluble silicate (as $Na_2O,2SiO_2$)	1 - 4%
Zeolite (as $NaA1SiO_4$)	24 - 34%
Sodium sulfate (as Na_2SO_4)	4 - 10%
Sodium citrate/citric acid (as $C_6H_5Na_3O_7/C_6H_8O_7$)	0 - 15%
Carboxymethylcellulose	0 - 2%
Polymers (e.g. maleic/acrylic acid copolymer, PVP, PEG)	1 - 6%
Enzymes (calculated as pure enzyme protein)	0.0001 - 0.1%
Minor ingredients (e.g. suds suppressors, perfume)	0 - 5%

3) A detergent composition formulated as a granulate having a bulk density of at least 600 g/l comprising

Linear alkylbenzenesulfonate (calculated as acid)	5 - 9%
Alcohol ethoxylate (e.g. C_{12-15} alcohol, 7 EO)	7 - 14%
Soap as fatty acid (e.g. C_{16-22} fatty acid)	1 - 3%
Sodium carbonate (as Na_2CO_3)	10 - 17%
Soluble silicate (as $Na_2O,2SiO_2$)	3 - 9%
Zeolite (as $NaA1SiO_4$)	23 - 33%
Sodium sulfate (as Na_2SO4)	0 - 4%
Sodium perborate (as $NaBO_3.H_2O$)	8 - 16%

TAED	2 - 8%
Phosphonate (e.g. EDTMPA)	0 - 1%
Carboxymethylcellulose	0 - 2%
Polymers (e.g. maleic/acrylic acid copolymer, PVP, PEG)	0 - 3%
Enzymes (calculated as pure enzyme protein)	0.0001 - 0.1%
Minor ingredients (e.g. suds suppressors, perfume, optical brightener)	0 - 5%

4) A detergent composition formulated as a granulate having a bulk density of at least 600 g/l comprising

Linear alkylbenzenesulfonate (calculated as acid)	8 - 12%
Alcohol ethoxylate (e.g. C_{12-15} alcohol, 7 EO)	10 - 25%
Sodium carbonate (as Na_2CO_3)	14 - 22%
Soluble silicate (as $Na_2O,2SiO_2$)	1 - 5%
Zeolite (as $NaAlSiO_4$)	25 - 35%
Sodium sulfate (as Na_2SO_4)	0 - 10%
Carboxymethylcellulose	0 - 2%
Polymers (e.g. maleic/acrylic acid copolymer, PVP, PEG)	1 - 3%
Enzymes (calculated as pure enzyme protein)	0.0001 - 0.1%
Minor ingredients (e.g. suds suppressors, perfume)	0 - 5%

5) An aqueous liquid detergent composition comprising

Linear alkylbenzenesulfonate (calculated as acid)	15 - 21%
Alcohol ethoxylate (e.g. C_{12-15} alcohol, 7 EO or C_{12-15} alcohol, 5 EO)	12 - 18%
Soap as fatty acid (e.g. oleic acid)	3 - 13%
Alkenylsuccinic acid (C_{12-14})	0 - 13%

Aminoethanol	8 - 18%
Citric acid	2 - 8%
Phosphonate	0 - 3%
Polymers (e.g. PVP, PEG)	0 - 3%
Borate (as B_4O_7)	0 - 2%
Ethanol	0 - 3%
Propylene glycol	8 - 14%
Enzymes (calculated as pure enzyme protein)	0.0001 - 0.1%
Minor ingredients (e.g. dispersants, suds suppressors, perfume, optical brightener)	0 - 5%

6) An aqueous structured liquid detergent composition comprising

Linear alkylbenzenesulfonate (calculated as acid)	15 - 21%
Alcohol ethoxylate (e.g. C_{12-15} alcohol, 7 EO, or C_{12-15} alcohol, 5 EO)	3 - 9%
Soap as fatty acid (e.g. oleic acid)	3 - 10%
Zeolite (as $NaAlSiO_4$)	14 - 22%
Potassium citrate	9 - 18%
Borate (as B_4O_7)	0 - 2%
Carboxymethylcellulose	0 - 2%
Polymers (e.g. PEG, PVP)	0 - 3%
Anchoring polymers such as, e.g., lauryl methacrylate/acrylic acid copolymer; molar ratio 25:1; MW 3800	0 - 3%
Glycerol	0 - 5%
Enzymes (calculated as pure enzyme protein)	0.0001 - 0.1%
Minor ingredients (e.g. dispersants, suds suppressors, perfume, optical brighteners)	0 - 5%

7) A detergent composition formulated as a granulate having a bulk density of at least 600 g/l comprising

Fatty alcohol sulfate	5 - 10%
Ethoxylated fatty acid monoethanol-amide	3 - 9%
Soap as fatty acid	0 - 3%
Sodium carbonate (as Na_2CO_3)	5 - 10%
Soluble silicate (as $Na_2O,2SiO_2$)	1 - 4%
Zeolite (as $NaAlSiO_4$)	20 - 40%
Sodium sulfate (as Na_2SO_4)	2 - 8%
Sodium perborate (as $NaBO_3.H_2O$)	12 - 18%
TAED	2 - 7%
Polymers (e.g. maleic/acrylic acid copolymer, PEG)	1 - 5%
Enzymes (calculated as pure enzyme protein)	0.0001 - 0.1%
Minor ingredients (e.g. optical brightener, suds suppressors, perfume)	0 - 5%

8) A detergent composition formulated as a granulate comprising

Linear alkylbenzenesulfonate (calculated as acid)	8 - 14%
Ethoxylated fatty acid monoethanol-amide	5 - 11%
Soap as fatty acid	0 - 3%
Sodium carbonate (as Na_2CO_3)	4 - 10%
Soluble silicate (as $Na_2O,2SiO_2$)	1 - 4%
Zeolite (as $NaAlSiO_4$)	30 - 50%
Sodium sulfate (as Na_2SO_4)	3 - 11%
Sodium citrate (as $C_6H_5Na_3O_7$)	5 - 12%
Polymers (e.g. PVP, maleic/acrylic acid copolymer, PEG)	1 - 5%
Enzymes (calculated as pure enzyme protein)	0.0001 - 0.1%
Minor ingredients (e.g. suds suppressors, perfume)	0 - 5%

9) A detergent composition formulated as a granulate comprising

Linear alkylbenzenesulfonate (calculated as acid)	6 - 12%
Nonionic surfactant	1 - 4%
Soap as fatty acid	2 - 6%
Sodium carbonate (as Na_2CO_3)	14 - 22%
Zeolite (as $NaAlSiO_4$)	18 - 32%
Sodium sulfate (as Na_2SO_4)	5 - 20%
Sodium citrate (as $C_6H_5Na_3O_7$)	3 - 8%
Sodium perborate (as $NaBO_3.H_2O$)	4 - 9%
Bleach activator (e.g. NOBS or TAED)	1 - 5%
Carboxymethylcellulose	0 - 2%
Polymers (e.g. polycarboxylate or PEG)	1 - 5%
Enzymes (calculated as pure enzyme protein)	0.0001 - 0.1%
Minor ingredients (e.g. optical brightener, perfume)	0 - 5%

10) An aqueous liquid detergent composition comprising

Linear alkylbenzenesulfonate (calculated as acid)	15 - 23%
Alcohol ethoxysulfate (e.g. C_{12-15} alcohol, 2-3 EO)	8 - 15%
Alcohol ethoxylate (e.g. C_{12-15} alcohol, 7 EO, or C_{12-15} alcohol, 5 EO)	3 - 9%
Soap as fatty acid (e.g. lauric acid)	0 - 3%
Aminoethanol	1 - 5%
Sodium citrate	5 - 10%
Hydrotrope (e.g. sodium toluensulfonate)	2 - 6%
Borate (as B_4O_7)	0 - 2%
Carboxymethylcellulose	0 - 1%
Ethanol	1 - 3%
Propylene glycol	2 - 5%

Enzymes (calculated as pure enzyme protein)	0.0001 - 0.1%
Minor ingredients (e.g. polymers, dispersants, perfume, optical brighteners)	0 - 5%

11) An aqueous liquid detergent composition comprising

Linear alkylbenzenesulfonate (calculated as acid)	20 - 32%
Alcohol ethoxylate (e.g. C_{12-15} alcohol, 7 EO, or C_{12-15} alcohol, 5 EO)	6 - 12%
Aminoethanol	2 - 6%
Citric acid	8 - 14%
Borate (as B_4O_7)	1 - 3%
Polymer (e.g. maleic/acrylic acid copolymer, anchoring polymer such as, e.g., lauryl methacrylate/acrylic acid copolymer)	0 - 3%
Glycerol	3 - 8%
Enzymes (calculated as pure enzyme protein)	0.0001 - 0.1%
Minor ingredients (e.g. hydrotropes, dispersants, perfume, optical brighteners)	0 - 5%

12) A detergent composition formulated as a granulate having a bulk density of at least 600 g/l comprising

Anionic surfactant (linear alkylbenzenesulfonate, alkyl sulfate, alpha-olefinsulfonate, alpha-sulfo fatty acid methyl esters, alkanesulfonates, soap)	25 - 40%
Nonionic surfactant (e.g. alcohol ethoxylate)	1 - 10%
Sodium carbonate (as Na_2CO_3)	8 - 25%
Soluble silicates (as Na_2O, $2SiO_2$)	5 - 15%
Sodium sulfate (as Na_2SO_4)	0 - 5%
Zeolite (as $NaAlSiO_4$)	15 - 28%
Sodium perborate (as $NaBO_3.4H_2O$)	0 - 20%

Bleach activator (TAED or NOBS)	0 - 5%
Enzymes (calculated as pure enzyme protein)	0.0001 - 0.1%
Minor ingredients (e.g. perfume, optical brighteners)	0 - 3%

13) Detergent formulations as described in 1) - 12) wherein all or part of the linear alkylbenzenesulfonate is replaced by (C_{12}-C_{18}) alkyl sulfate.

14) A detergent composition formulated as a granulate having a bulk density of at least 600 g/l comprising

(C_{12}-C_{18}) alkyl sulfate	9 - 15%
Alcohol ethoxylate	3 - 6%
Polyhydroxy alkyl fatty acid amide	1 - 5%
Zeolite (as $NaAlSiO_4$)	10 - 20%
Layered disilicate (e.g. SK56 from Hoechst)	10 - 20%
Sodium carbonate (as Na_2CO_3)	3 - 12%
Soluble silicate (as $Na_2O,2SiO_2$)	0 - 6%
Sodium citrate	4 - 8%
Sodium percarbonate	13 - 22%
TAED	3 - 8%
Polymers (e.g. polycarboxylates and PVP=	0 - 5%
Enzymes (calculated as pure enzyme protein)	0.0001 - 0.1%
Minor ingredients (e.g. optical brightener, photo bleach, perfume, suds suppressors)	0 - 5%

15) A detergent composition formulated as a granulate having a bulk density of at least 600 g/l comprising

(C_{12}-C_{18}) alkyl sulfate	4 - 8%
Alcohol ethoxylate	11 - 15%

Soap	1 - 4%
Zeolite MAP or zeolite A	35 - 45%
Sodium carbonate (as Na_2CO_3)	2 - 8%
Soluble silicate (as $Na_2O,2SiO_2$)	0 - 4%
Sodium percarbonate	13 - 22%
TAED	1 - 8%
Carboxymethyl cellulose	0 - 3%
Polymers (e.g. polycarboxylates and PVP)	0 - 3%
Enzymes (calculated as pure enzyme protein)	0.0001 - 0.1%
Minor ingredients (e.g. optical brightener, phosphonate, perfume)	0 - 3%

16) Detergent formulations as described in 1) - 15) which contain a stabilized or encapsulated peracid, either as an additional component or as a substitute for already specified bleach systems.

17) Detergent compositions as described in 1), 3), 7), 9) and 12) wherein perborate is replaced by percarbonate.

18) Detergent compositions as described in 1), 3), 7), 9), 12), 14) and 15) which additionally contain a manganese catalyst. The manganese catalyst may, e.g., be one of the compounds described in "Efficient manganese catalysts for low-temperature bleaching", Nature 369, 1994, pp. 637-639.

19) Detergent composition formulated as a nonaqueous detergent liquid comprising a liquid nonionic surfactant such as, e.g., linear alkoxylated primary alcohol, a builder system (e.g. phosphate), enzyme and alkali. The detergent may also comprise anionic surfactant and/or a bleach system.

The α-amylase variant of the invention may be incorporated in concentrations conventionally employed in detergents. It is at present contemplated that, in the detergent composition of the invention, the α-amylase may be added in an amount correspon-

ding to 0.00001-1 mg (calculated as pure enzyme protein) of α-amylase per liter of wash liquor.

Dishwashing Composition

The dishwashing detergent composition comprises a surfactant which may be anionic, non-ionic, cationic, amphoteric or a mixture of these types. The detergent will contain 0-90% of non-ionic surfactant such as low- to non-foaming ethoxylated propoxylated straight-chain alcohols.

The detergent composition may contain detergent builder salts of inorganic and/or organic types. The detergent builders may be subdivided into phosphorus-containing and non-phosphorus-containing types. The detergent composition usually contains 1-90% of detergent builders.

Examples of phosphorus-containing inorganic alkaline detergent builders, when present, include the water-soluble salts especially alkali metal pyrophosphates, orthophosphates, and polyphosphates. An example of phosphorus-containing organic alkaline detergent builder, when present, includes the water-soluble salts of phosphonates. Examples of non-phosphorus-containing inorganic builders, when present, include water-soluble alkali metal carbonates, borates and silicates as well as the various types of water-insoluble crystalline or amorphous alumino silicates of which zeolites are the best-known representatives.

Examples of suitable organic builders include the alkali metal, ammonium and substituted ammonium, citrates, succinates, malonates, fatty acid sulphonates, carboxymetoxy succinates, ammonium polyacetates, carboxylates, polycarboxylates, aminopolycarboxylates, polyacetyl carboxylates and polyhydroxsulphonates.

Other suitable organic builders include the higher molecular weight polymers and co-polymers known to have builder properties, for example appropriate polyacrylic acid, polymaleic and polyacrylic/polymaleic acid copolymers and their salts.

The dishwashing detergent composition may contain bleaching agents of the chlorine/bromine-type or the oxygen-type. Examples of inorganic chlorine/bromine-type bleaches are lithium, sodium or calcium hypochlorite and hypobromite as well as chlorinated trisodium phosphate. Examples of organic chlorine/bromine-type bleaches are heterocyclic N-bromo and N-chloro imides such as trichloroisocyanuric, tribromoisocyanuric, dibromoisocyanuric and dichloroisocyanuric acids, and salts thereof with water-solubilizing cations such as potassium and sodium. Hydantoin compounds are also suitable.

The oxygen bleaches are preferred, for example in the form of an inorganic persalt, preferably with a bleach precursor or as a peroxy acid compound. Typical examples of suitable peroxy bleach compounds are alkali metal perborates, both tetrahydrates and monohydrates, alkali metal percarbonates, persilicates and perphosphates. Preferred activator materials are TAED and glycerol triacetate.

The dishwashing detergent composition of the invention may be stabilized using conventional stabilizing agents for the enzyme(s), e.g. a polyol such as e.g.propylene glycol, a sugar or a sugar alcohol, lactic acid, boric acid, or a boric acid derivative, e.g. an aromatic borate ester.

The dishwashing detergent composition of the invention may also contain other conventional detergent ingredients, e.g. deflocculant material, filler material, foam depressors, anti-corrosion agents, soil-suspending agents, sequestering agents, anti-soil redeposition agents, dehydrating agents, dyes, bactericides, fluorescers, thickeners and perfumes.

Finally, the α-amylase variant of the invention may be used in conventional dishwashing detergents, e.g. in any of the following patent publications:

EP 518719, EP 518720, EP 518721, EP 516553, EP 516554,

EP 516555, GB 2200132, DE 3741617, DE 3727911, DE 4212166, DE 4137470, DE 3833047, WO 93/17089, DE 4205071, WO 52/09680, WO 93/18129, WO 93/04153, WO 92/06157, WO 92/08777, EP 429124, WO 93/21299, US 5141664, EP 561452, EP 561446, GB 2234980, WO 93/03129, EP 481547, EP 530870, EP 533239, EP 554943, EP 346137, US 5112518, EP 318204, EP 318279, EP 271155, EP 271156, EP 346136, GB 2228945, CA 2006687, WO 93/25651, EP 530635, EP 414197, US 5240632.

EXAMPLES

EXAMPLE 1

Example on Homology building of TERM

The overall homology of the *B. licheniformis* α-amylase (in the following referred to as TERM) to other Termamyl-like α-amylases is high and the percent similarity is extremely high. The similarity calculated for TERM to BSG (the *B. stearothermophilus* α-amylase with SEQ ID NO 6), and BAN (the *B. amyloliquefaciens* α-amylase with SEQ ID NO 4) using the University of Wisconsin Genetics Computer Group's program GCG gave 89% and 78%, respectively. TERM has a deletion of 2 residues between residue G180 and K181 compared to BAN and BSG. BSG has a deletion of 3 residues between G371 and I372 in comparison with BAN and TERM. Further BSG has a C-terminal extension of more than 20 residues compared to BAN and TERM. BAN has 2 residues less and TERM has one residue less in the N-terminal compared to BSG.

The structure of the *B. licheniformis* (TERM) and of the *B. amyloliquefaciens* α-amylase (BAN), respectively, was model built on the structure disclosed in Appendix 1 herein. The structure of other Termamyl-like α-amylases (e.g. those disclosed herein) may be built analogously.

In comparison with the α-amylase used for elucidating the present structure, TERM differs in that it lacks two residues around 178-182. In order to compensate for this in the model structure, the HOMOLOGY program from BIOSYM was used to substitute the residues in equivalent positions in the structure (not only structurally conserved regions) except for the deletion point. A peptide bond was established between G179(G177) and K180(K180) in TERM(BAN). The close structural relationship between the solved structure and the model structure (and thus the validity of the latter) is indicated by the presence of only very few atoms found to be too close together in the model.

To this very rough structure of TERM was then added all waters (605) and ions (4 Calcium and 1 Sodium) from the solved structure (Appendix 1) at the same coordinates as for said solved structure using the INSIGHT program. This could be done with only few overlaps - in other words with a very nice fit. This model structure were then minimized using 200 steps of Steepest descent and 600 steps of Conjugated gradient (see Brooks et al 1983, J. Computational Chemistry 4, p.187-217). The minimized structure was then subjected to molecular dynamics, 5ps heating followed by up to 200ps equilibration but more than 35ps. The dynamics as run with the Verlet algorithm and the equilibration temperature 300K were kept using the Behrendsen coupling to a waterbath (Berendsen et. al., 1984, J. Chemical Physics 81, p. 3684-3690). Rotations and translations were removed every picosecond. The potential energy became stable after appr. 35ps equilibration. A mean dynamics structure was extracted and can be used for further analysis.

EXAMPLE 2

Determination of residues within 10Å from the ions present in the solved structure

The coordinates of Appendix 1 are read into the INSIGHT program provided by BIOSYM tecnologies. The spatial coordinates are

presented showing the bonds between the atoms. The ions are presented as well as the water atoms. The program package part of creating subset are used to create a 10Å subset around the Calcium and the Sodium ions in the structure using the command ZONE. All residues having an atom within the 10Å are compiled and written out by the LIST MOLECULE command. By giving the ions the name ium in the coordinate file a 10Å sphere around all atoms called ium is compiled. The specific residues identified in this manner are given further above in the section entitled "Ca^{2+} dependency".

EXAMPLE 3

Determination of cavities in the solved structure (Appendix 1)

The solved structure exhibits many internal holes and cavities. When analysing for such cavities the Connolly program is normally used (Lee, B. and Richards, F.M. (1971) J. Mol. Biol. 55,p. 379-400). The program uses a probe with radius to search the external and internal surface of the protein. The smallest hole observable in this way has the probe radius.

To analyse the solved structure a modified version of the Connolly program included in the program of INSIGHT were used. First the water molecules and the ions were removed by unmerging these atoms from the solved structure. By using the command MOLECULE SURFACE SOLVENT the solvent accessible surface area were calculated for all atoms and residues using a probe radius of 1.4Å, and displayed on the graphics screen together with the model of the solved structure. The internal cavities where then seen as dot surfaces with no connections to external surface.

Mutant suggestions for filling out the holes are given in the specification (in the section entitled "Variants with increased thermostability and/or altered temperature optimum"). By using the homology build structures or/and the sequence alignment

mutations for the homologous structures of TERM and BSG and BAN can be made.

EXAMPLE 4

Construction of Termamyl™ variants in accordance with the invention

Termamyl (SEQ ID NO. 2) is expressed in *B. subtilis* from a plasmid denoted pDN1528. This plasmid contains the complete gene encoding Termamyl, *amyL*, the expression of which is directed by its own promoter. Further, the plasmid contains the origin of replication, *ori*, from plasmid pUB110 and the *cat* gene from plasmid pC194 conferring resistance towards chloramphenicol. pDN1528 is shown in Fig. 9.

A specific mutagenesis vector containing a major part of the coding region of SEQ ID NO 1 was prepared. The important features of this vector, denoted pJeEN1, include an origin of replication derived from the pUC plasmids, the *cat* gene conferring resistance towards chloramphenicol, and a frameshift-containing version of the *bla* gene, the wild type of which normally confers resistance towards ampicillin (amp^R phenotype). This mutated version results in an amp^S phenotype. The plasmid pJeEN1 is shown in Fig. 10, and the *E. coli* origin of replication, *ori*, *bla*, *cat* , the 5'-truncated version of the Termamyl amylase gene, and selected restriction sites are indicated on the plasmid.

Mutations are introduced in *amyL* by the method described by Deng and Nickoloff (1992, Anal. Biochem. 200, pp. 81-88) except that plasmids with the "selection primer" (primer #6616; see below) incorporated are selected based on the amp^R phenotype of transformed *E. coli* cells harboring a plasmid with a repaired *bla* gene, instead of employing the selection by restriction enzyme digestion outlined by Deng and Nickoloff. Chemicals and enzymes used for the mutagenesis were obtained from the

Chameleon™ mutagenesis kit from Stratagene (catalogue number 200509).

After verification of the DNA sequence in variant plasmids, the truncated gene, containing the desired alteration, is subcloned into pDN1528 as a *Pst*I-*Eco*RI fragment and transformed into a protease- and amylase-depleted *Bacillus subtilis* strain in order to express the variant enzyme.

The Termamyl variant V54W was constructed by the use of the following mutagenesis primer (written 5′ to 3′, left to right):

PG GTC GTA GGC ACC GTA GCC CCA ATC CGC TTG

The Termamyl variant A52W + V54W was constructed by the use of the following mutagenesis primer (written 5′ to 3′, left to right):

PG GTC GTA GGC ACC GTA GCC CCA ATC CCA TTG GCT CG

Primer #6616 (written 5′ to 3′, left to right; P denotes a 5′ phosphate):

P CTG TGA CTG GTG AGT ACT CAA CCA AGT C

EXAMPLE 5

Saccharification in the presence of "residual" α-amylase activity

Two appropriate Termamyl variants with altered specificity were evaluated by saccharifying a DE 10 (DE = dextrose equivalent) maltodextrin substrate with *A. niger* glucoamylase and *B. acidopullulyticus* pullulanase under conditions where the variant amylase was active.

<u>Saccharification</u>: Substrates for saccharification were prepared by dissolving 230 g DE 10 spray-dried maltodextrin, prepared

from common corn starch, in 460 ml boiling deionized water and adjusting the dry substance (DS) content to approximately 30% w/w. The pH was adjusted to 4.7 (measured at 60°C) and aliquots of substrate corresponding to 15 g dry weight were transferred to 50 ml blue cap glass flasks.

The flasks were then placed in a shaking water bath equilibrated at 60°C, and the enzymes added. The pH was readjusted to 4.7 where necessary.

The following enzymes were used:

Glucoamylase:	AMG™ (Novo Nordisk A/S); dosage 0.18 AG/g DS
Pullulanase:	Promozyme™ (Novo Nordisk A/S); dosage 0.06 PUN/g DS
α-Amylases:	Termamyl™ (Novo Nordisk A/S); dosage 60 NU/g DS
	Termamyl variant V54W; dosage 60 NU/g DS
	Termamyl variant V54W + A52W; dosage 60 NU/g DS

2 ml samples were taken periodically. The pH of each sample was adjusted to about 3.0, and the sample was then heated in a boiling water bath for 15 minutes to inactivate the enzymes. After cooling, the samples were treated with approximately 0.1 g mixed-bed ion exchange resin (BIO-Rad 501-X (D)) for 30 minutes on a rotary mixer and then filtered. The carbohydrate composition of each sample was determined by HPLC. The following results were obtained after 72 hours [DP_n denotes a dextrose (D-glucose) oligomer with n glucose units]:

α-amylase	%DP_1	%DP_2	%DP_3	%DP_4
None (control)	95.9	2.8	0.4	1.0
V54W	96.0	2.9	0.4	0.8
V54W + A52W	95.9	2.8	0.4	0.8
Termamyl™	95.6	2.8	0.8	0.8

It can be seen from the above results that compared with the control (no α-amylase activity present during liquefaction), the presence of α-amylase activity from variants V54W and V54W + A52W did not lead to elevated panose (DP_3) levels. In contrast, Termamyl α-amylase activity resulted in higher levels of panose and a subsequent loss of D-glucose (DP_1) yield.

Thus, if α-amylase variants V54W or V54W + A52W are used for starch liquefaction, it will not be necessary to inactivate the residual α-amylase activity before the commencement of saccharification.

EXAMPLE 6

Calcium-binding affinity of α-amylase variants of the invention

Unfolding of amylases by exposure to heat or to denaturants such as guanidine hydrochloride is accompanied by a decrease in fluorescence. Loss of calcium ions leads to unfolding, and the affinity of α-amylases for calcium can be measured by fluorescence measurements before and after incubation of each α-amylase (e.g. at a concentration of 10 μg/ml) in a buffer (e.g. 50 mM HEPES, pH 7) with different concentrations of calcium (e.g. in the range of 1 μM-100 mM) or of EGTA (e.g. in the range of 1-1000 μM) [EGTA = 1,2-di(2-aminoethoxy)ethane-*N,N,N',N'*-tetraacetic acid] for a sufficiently long period of time (such as 22 hours at 55°C).

The measured fluorescence F is composed of contributions form the folded and unfolded forms of the enzyme. The following equation can be derived to describe the dependence of F on calcium concentration ([Ca]):

$$F = [Ca]/(K_{diss} + [Ca])(\alpha_N - \beta_N \log([Ca])) + K_{diss}/(K_{diss} + [Ca])(\alpha_U - \beta_U \log([Ca]))$$

where α_N is the fluorescence of the native (folded) form of the enzyme, β_N is the linear dependence of α_N on the logarithm of

the calcium concentration (as observed experimentally), α_U is the fluorescence of the unfolded form and β_U is the linear dependence of α_U on the logarithm of the calcium concentration. K_{diss} is the apparent calcium-binding constant for an equilibrium process as follows:

$$N\text{-}Ca \overset{K_{diss}}{\leftrightarrow} U + Ca \quad (N = \text{native enzyme; } U = \text{unfolded enzyme})$$

In fact, unfolding proceeds extremely slowly and is irreversible. The rate of unfolding is a dependent on calcium concentration, and the dependency for a given α-amylase provides a measure of the Ca-binding affinity of the enzyme. By defining a standard set of reaction conditions (e.g. 22 hours at 55°C), a meaningful comparison of K_{diss} for different α-amylases can be made. The calcium dissociation curves for α-amylases in general can be fitted to the equation above, allowing determination of the corresponding values of K_{diss}.

The following values for K_{diss} were obtained for a parent Termamyl-like α-amylase having the amino acid sequence shown in SEQ ID No. 1 of WO 95/26397 and for the indicated variant thereof according to the invention:

α-Amylase	K_{diss} (mol/l)
L351C + M430C + T183* + G184*	1.7 (±0.5) x 10^{-3}
Parent	3.5 (±1.1) x 10^{-1}

It is apparent from the above that the calcium-binding affinity of the variant in question binds calcium significantly more strongly than the parent, and thereby has a correspondingly lower calcium dependency than the parent.

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SEQUENCE LISTING

In the following SEQ ID Nos. 1, 3, 5 the 5', coding sequence and 3' sequence of the relevant α-amylase genes are illustrated. The 5' sequence is the first separate part of the sequence written with lower case letters, the coding sequence is the intermediate part of the sequence, where the signal sequence is written with lower case letters and the sequence encoding the mature α-amylase is written with upper case letters, and the 3' sequence is the third separate part of the sequence written with lower case letters.

SEQ ID No. 1

cggaagattggaagtacaaaaataagcaaaagattgtcaatcatgtcatgagccatgcgg-
gagacggaaaaatcgtctta atgcacgatatttatgcaacgttcgcagatgctgctgaa-
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TTGGCTGAACACGGTATTACTGCCGTCTGGATTCCCCCGGCATATAA GGGAACGAGC-
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ATTCCCGCGACATTAACGTTTACGGGGAT GTGGTCATCAACCACAAAGGCGGCGCTGA-
TGCGACCGAAGATGTAACCGCGGTTGAAGTCGATCCCGCTGACCGCAACCG CGTAATTT-
CAGGAGAACACCTAATTAAAGCCTGGACACATTTTCATTTTCCGGGGCGCGGCAGCACATA-
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GCTGAACCGCATCTATAAGTTTCAAGGAAAG GCTTGGGATTGGGAAGTTTCCAATGAA-
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GTGCC GCTTCATTATCAGTTCCATGCTGCATCGACACAGGGAGGCGGCTATGATATGAG-
GAAATTGCTGAACGGTACGGTCGTTT CCAAGCATCCGTTGAAATCGGTTACATTTGTCG-
ATAACCATGATACACAGCCGGGGCAATCGCTTGAGTCGACTGTCCAA ACATGGTTTAAG-
CCGCTTGCTTACGCTTTTATTCTCACAAGGGAATCTGGATACCCTCAGGTTTTCTACGGG-
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TGAACCGATCTTAAAAGCGAGAAAACAGT ATGCGTACGGAGCACAGCATGATTATTTCGAC-
CACCATGACATTGTCGGCTGGACAAGGGAAGGCGACAGCTCGGTTGCA AATTCAGGTTTGG-
CGGCATTAATAACAGACGGACCCGGTGGGGCAAAGCGAATGTATGTCGGCCGGCA-
AAACGCCGGTGA GACATGGCATGACATTACCGGAAACCGTTCGGAGCCGGTTGTCATCA-
ATTCGGAAGGCTGGGGAGAGTTTCACGTAAACG GCGGGTCGGTTTCAATTTATGTTCAAA-
GATAG

aagagcagagaggacggatttcctgaaggaaatccgtttttttatttt

SEQ ID No. 2

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VQR

SEQ ID No. 3

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TGAAAATCATGACACACAGCCGGGACAGTCATTGGAATCGACAGTCC AAACTTGGTTTAA-
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CACCCGGATGTGATCGGATGGACGAGGGAAGGTGACAGCTCCGCCG CCAA-
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SEQ ID No. 4

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SEQ ID No. 5

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CCGCCCGCTTACAA AGGAACAAGCCGCAGCGACGTAGGGTACGGAGTATACGACTTGTA-
TGACCTCGGCGAATTCAATCAAAAAGGGACCGTCC GCACAAAATACGGAACAAAAGCTC-
AATATCTTCAAGCCATTCAAGCCGCCCACGCCGCTGGAATGCAAGTGTACGCCGAT GTC-
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CCGTCCGACCGCAACCA AGAAATCTCGGGCACCTATCAAATCCAAGCATGGACGAAATT-
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GGCAAAGCGTGGGATTGGGAAGTAGACACGGAAAACGGAAACTATGACTACTTAATGTAT-
GCCGACCTTGATATGGATCA TCCCGAAGTCGTGACCGAGCTGAAAAACTGGGGGAAATG-
GTATGTCAACACAACGAACATTGATGGGTTCCGGCTTGATG CCGTCAAGCATATTAAGT-
TCAGTTTTTTTCCTGATTGGTTGTCGTATGTGCGTTCTCAGACTGGCAAGCCGCTATTTACC
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GGAACGATGTCTTTGTTTGA TGCCCCGTTACACAACAAATTTTATACCGCTTCCAAATCAG-
GGGGCGCATTTGATATGCGCACGTTAATGACCAATACTC TCATGAAAGATCAAC-
CGACATTGGCCGTCACCTTCGTTGATAATCATGACACCGAACCCGGCCAAGCGC-
TGCAGTCATGG GTCGACCCATGGTTCAAACCGTTGGCTTACGCCTTTATTCTAACTCGG-
CAGGAAGGATACCCGTGCGTCTTTTATGGTGA CTATTATGGCATTCCACAATATAACAT-
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tgcctgcga

SEQ ID No. 6

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KAQYLQAIQAAHAAGMQVYADVVFDHKGGADGTEWVDAVE
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FDGVDWDESRKLSRIYKFRGIGKAWDWEVDTENGNYDYLM
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SEQ ID No. 10

1 ATPADWRSQS IYFLLTDRFA RTDGSTTATC
31 NTADQKYCGG TWQGIIDKLD YIQGMGFTAI
61 WITPVTAQLP QTTAYGDAYH GYWQQDIYSL
91 NENYGTADDL KALSSALHER GMYLMVDVVA

121 NHMGYDGAGS SVDYSVFKPF SSQDYFHPFC
151 FIQNYEDQTQ VEDCWLGDNT VSLPDLDTTK
181 DVVKNEWYDW VGSLVSNYSI DGLRIDTVKH
211 VQKDFWPGYN KAAGVYCIGE VLDGDPAYTC
241 PYQNVMDGVL NYPIYYPLLN AFKSTSGSMD
271 DLYNMINTVK SDCPDSTLLG TFVENHDNPR
301 FASYTNDIAL AKNVAAFIIL NDGIPIIYAG
331 QEQHYAGGND PANREATWLS GYPTDSELYK
361 LIASANAIRN YAISKDTGFV TYKNWPIYKD
391 DITIAMRKGT DGSQIVTILS NKGASGDSYT
421 LSLSGAGYTA GQQLTEVIGC TTVTVGSDGN
451 VPVPMAGGLP RVLYPTEKLA GSKICSSS

ATOM	1	CB	VAL	A	1	11.902	27.157	22.095	1.00	23.86	6
ATOM	2	CG1	VAL	A	1	12.302	27.494	20.658	1.00	24.08	6
ATOM	3	CG2	VAL	A	1	10.659	27.948	22.511	1.00	26.37	6
ATOM	4	C	VAL	A	1	13.030	25.096	22.743	1.00	19.54	6
ATOM	5	O	VAL	A	1	13.191	25.013	23.967	1.00	19.86	8
ATOM	6	N	VAL	A	1	10.702	25.241	23.415	1.00	20.28	7
ATOM	7	CA	VAL	A	1	11.659	25.658	22.335	1.00	20.25	6
ATOM	8	N	ASN	A	2	13.867	24.729	21.802	1.00	18.39	7
ATOM	9	CA	ASN	A	2	15.168	24.197	22.212	1.00	16.73	6
ATOM	10	CB	ASN	A	2	15.836	23.657	20.945	1.00	16.09	6
ATOM	11	CG	ASN	A	2	15.219	22.336	20.451	1.00	15.33	6
ATOM	12	OD1	ASN	A	2	14.707	21.549	21.252	1.00	15.28	8
ATOM	13	ND2	ASN	A	2	15.283	22.082	19.151	1.00	12.41	7
ATOM	14	C	ASN	A	2	15.969	25.334	22.767	1.00	15.71	6
ATOM	15	O	ASN	A	2	15.903	26.435	22.198	1.00	16.02	8
ATOM	16	N	GLY	A	3	16.720	25.198	23.833	1.00	14.56	7
ATOM	17	CA	GLY	A	3	17.541	26.305	24.331	1.00	13.21	6
ATOM	18	C	GLY	A	3	18.940	26.211	23.671	1.00	12.14	6
ATOM	19	O	GLY	A	3	19.498	25.153	23.302	1.00	11.92	8
ATOM	20	N	THR	A	4	19.503	27.368	23.499	1.00	11.28	7
ATOM	21	CA	THR	A	4	20.829	27.555	22.912	1.00	10.96	6
ATOM	22	CB	THR	A	4	20.721	27.878	21.400	1.00	11.09	6
ATOM	23	OG1	THR	A	4	19.920	26.828	20.782	1.00	12.31	8
ATOM	24	CG2	THR	A	4	22.048	27.933	20.693	1.00	8.99	6
ATOM	25	C	THR	A	4	21.584	28.664	23.663	1.00	10.56	6
ATOM	26	O	THR	A	4	21.080	29.743	23.866	1.00	9.98	8
ATOM	27	N	LEU	A	5	22.809	28.376	24.092	1.00	10.63	7
ATOM	28	CA	LEU	A	5	23.700	29.291	24.818	1.00	10.69	6
ATOM	29	CB	LEU	A	5	24.515	28.477	25.789	1.00	9.31	6
ATOM	30	CG	LEU	A	5	25.429	28.946	26.864	1.00	10.96	6
ATOM	31	CD1	LEU	A	5	24.887	30.150	27.608	1.00	9.46	6
ATOM	32	CD2	LEU	A	5	25.608	27.802	27.884	1.00	10.55	6
ATOM	33	C	LEU	A	5	24.644	29.992	23.840	1.00	10.85	6
ATOM	34	O	LEU	A	5	25.047	29.453	22.799	1.00	10.85	8
ATOM	35	N	MET	A	6	25.031	31.217	24.123	1.00	10.88	7
ATOM	36	CA	MET	A	6	25.971	31.930	23.312	1.00	10.94	6
ATOM	37	CB	MET	A	6	25.455	33.143	22.507	1.00	12.97	6
ATOM	38	CG	MET	A	6	26.629	33.643	21.638	1.00	15.17	6
ATOM	39	SD	MET	A	6	26.027	34.480	20.185	1.00	19.39	16
ATOM	40	CE	MET	A	6	27.525	35.144	19.516	1.00	16.94	6
ATOM	41	C	MET	A	6	27.089	32.485	24.223	1.00	10.67	6
ATOM	42	O	MET	A	6	26.774	33.206	25.170	1.00	10.51	8
ATOM	43	N	GLN	A	7	28.325	32.133	23.911	1.00	10.34	7
ATOM	44	CA	GLN	A	7	29.440	32.727	24.681	1.00	10.20	6
ATOM	45	CB	GLN	A	7	30.696	31.910	24.617	1.00	9.41	6
ATOM	46	CG	GLN	A	7	31.967	32.632	25.053	1.00	10.26	6
ATOM	47	CD	GLN	A	7	33.280	31.914	25.027	1.00	9.15	6
ATOM	48	OE1	GLN	A	7	34.327	32.470	25.449	1.00	12.35	8
ATOM	49	NE2	GLN	A	7	33.359	30.714	24.570	1.00	6.58	7
ATOM	50	C	GLN	A	7	29.578	34.125	24.015	1.00	10.22	6
ATOM	51	O	GLN	A	7	29.856	34.167	22.786	1.00	10.30	8
ATOM	52	N	TYR	A	8	29.394	35.236	24.691	1.00	9.97	7
ATOM	53	CA	TYR	A	8	29.467	36.526	24.022	1.00	9.95	6
ATOM	54	CB	TYR	A	8	28.238	37.382	24.476	1.00	10.19	6
ATOM	55	CG	TYR	A	8	27.909	38.377	23.351	1.00	10.76	6
ATOM	56	CD1	TYR	A	8	27.180	37.983	22.222	1.00	11.00	6
ATOM	57	CE1	TYR	A	8	26.891	38.842	21.190	1.00	11.22	6
ATOM	58	CD2	TYR	A	8	28.340	39.698	23.424	1.00	10.96	6
ATOM	59	CE2	TYR	A	8	28.080	40.620	22.423	1.00	11.25	6
ATOM	60	CZ	TYR	A	8	27.358	40.156	21.312	1.00	11.62	6
ATOM	61	OH	TYR	A	8	27.114	41.063	20.294	1.00	11.87	8
ATOM	62	C	TYR	A	8	30.789	37.289	24.119	1.00	9.70	6
ATOM	63	O	TYR	A	8	30.918	38.427	24.563	1.00	9.67	8
ATOM	64	N	PHE	A	9	31.890	36.710	23.639	1.00	9.16	7
ATOM	65	CA	PHE	A	9	33.191	37.307	23.588	1.00	9.15	6
ATOM	66	CB	PHE	A	9	33.805	37.750	24.941	1.00	8.08	6
ATOM	67	CG	PHE	A	9	33.968	36.659	25.978	1.00	9.21	6
ATOM	68	CD1	PHE	A	9	35.239	36.125	26.240	1.00	10.15	6
ATOM	69	CD2	PHE	A	9	32.887	36.171	26.720	1.00	7.79	6
ATOM	70	CE1	PHE	A	9	35.440	35.161	27.245	1.00	10.23	6
ATOM	71	CE2	PHE	A	9	33.070	35.205	27.669	1.00	7.64	6
ATOM	72	CZ	PHE	A	9	34.313	34.698	27.962	1.00	8.17	6
ATOM	73	C	PHE	A	9	34.173	36.294	22.963	1.00	8.94	6
ATOM	74	O	PHE	A	9	33.903	35.102	22.918	1.00	8.65	8
ATOM	75	N	GLU	A	10	35.284	36.856	22.536	1.00	9.09	7
ATOM	76	CA	GLU	A	10	36.430	36.089	22.006	1.00	9.38	6
ATOM	77	CB	GLU	A	10	36.508	36.043	20.513	1.00	7.45	6
ATOM	78	CG	GLU	A	10	36.604	37.345	19.740	1.00	7.55	6
ATOM	79	CD	GLU	A	10	37.981	37.580	19.156	1.00	6.81	6
ATOM	80	OE1	GLU	A	10	38.145	38.544	18.397	1.00	8.43	8
ATOM	81	OE2	GLU	A	10	38.962	36.877	19.438	1.00	5.00	8
ATOM	82	C	GLU	A	10	37.636	36.715	22.737	1.00	9.90	6
ATOM	83	O	GLU	A	10	37.590	37.807	23.361	1.00	9.92	8
ATOM	84	N	TRP	A	11	38.791	36.059	22.729	1.00	10.15	7
ATOM	85	CA	TRP	A	11	39.980	36.551	23.407	1.00	10.35	6
ATOM	86	CB	TRP	A	11	41.182	35.619	23.186	1.00	9.98	6
ATOM	87	CG	TRP	A	11	42.271	35.940	24.181	1.00	11.61	6
ATOM	88	CD2	TRP	A	11	42.292	35.583	25.565	1.00	12.44	6
ATOM	89	CE2	TRP	A	11	43.516	36.063	26.103	1.00	12.84	6
ATOM	90	CE3	TRP	A	11	41.412	34.916	26.432	1.00	13.39	6
ATOM	91	CD1	TRP	A	11	43.446	36.606	23.915	1.00	11.78	6
ATOM	92	NE1	TRP	A	11	44.188	36.673	25.083	1.00	12.99	7
ATOM	93	CZ2	TRP	A	11	43.831	35.890	27.441	1.00	13.37	6
ATOM	94	CZ3	TRP	A	11	41.717	34.763	27.772	1.00	13.91	6
ATOM	95	CH2	TRP	A	11	42.946	35.256	28.280	1.00	14.23	6
ATOM	96	C	TRP	A	11	40.410	37.937	22.933	1.00	10.57	6
ATOM	97	O	TRP	A	11	40.843	38.709	23.797	1.00	10.47	8
ATOM	98	N	TYR	A	12	40.322	38.209	21.623	1.00	10.73	7
ATOM	99	CA	TYR	A	12	40.766	39.508	21.126	1.00	11.11	6
ATOM	100	CB	TYR	A	12	41.559	39.432	19.798	1.00	11.11	6
ATOM	101	CG	TYR	A	12	42.765	38.515	20.029	1.00	11.60	6
ATOM	102	CD1	TYR	A	12	42.605	37.158	19.704	1.00	11.95	6
ATOM	103	CE1	TYR	A	12	43.666	36.268	19.892	1.00	12.43	6
ATOM	104	CD2	TYR	A	12	43.985	38.951	20.540	1.00	11.48	6
ATOM	105	CE2	TYR	A	12	45.023	38.076	20.714	1.00	11.85	6
ATOM	106	CZ	TYR	A	12	44.870	36.749	20.388	1.00	12.61	6

Appendix 1

ATOM	107	OH	TYR	A	12	45.854	35.787	20.560	1.00	13.18	8
ATOM	108	C	TYR	A	12	39.687	40.574	20.991	1.00	11.38	6
ATOM	109	O	TYR	A	12	39.862	41.436	20.132	1.00	11.53	8
ATOM	110	N	THR	A	13	38.630	40.547	21.783	1.00	11.49	7
ATOM	111	CA	THR	A	13	37.651	41.656	21.700	1.00	11.50	6
ATOM	112	CB	THR	A	13	36.604	41.321	22.761	1.00	13.32	6
ATOM	113	OG1	THR	A	13	35.755	40.296	22.169	1.00	14.85	8
ATOM	114	CG2	THR	A	13	35.732	42.466	23.175	1.00	14.00	6
ATOM	115	C	THR	A	13	38.489	42.880	22.036	1.00	11.41	6
ATOM	116	O	THR	A	13	39.429	42.805	22.840	1.00	11.13	8
ATOM	117	N	PRO	A	14	38.254	44.015	21.408	1.00	11.47	7
ATOM	118	CD	PRO	A	14	37.184	44.144	20.397	1.00	11.68	6
ATOM	119	CA	PRO	A	14	38.979	45.243	21.611	1.00	11.44	6
ATOM	120	CB	PRO	A	14	38.477	46.296	20.569	1.00	11.60	6
ATOM	121	CG	PRO	A	14	37.352	45.564	19.896	1.00	11.77	6
ATOM	122	C	PRO	A	14	38.786	45.868	22.993	1.00	11.21	6
ATOM	123	O	PRO	A	14	37.703	45.785	23.618	1.00	11.15	8
ATOM	124	N	ASN	A	15	39.806	46.557	23.445	1.00	10.84	7
ATOM	125	CA	ASN	A	15	39.720	47.304	24.693	1.00	11.02	6
ATOM	126	CB	ASN	A	15	41.073	47.318	25.411	1.00	11.27	6
ATOM	127	CG	ASN	A	15	41.055	48.247	26.614	1.00	11.89	6
ATOM	128	OD1	ASN	A	15	40.008	48.358	27.277	1.00	12.57	8
ATOM	129	ND2	ASN	A	15	42.158	48.898	26.922	1.00	11.38	7
ATOM	130	C	ASN	A	15	39.240	48.737	24.377	1.00	11.05	6
ATOM	131	O	ASN	A	15	39.932	49.767	24.524	1.00	11.08	8
ATOM	132	N	ASP	A	16	38.008	48.835	23.905	1.00	10.98	7
ATOM	133	CA	ASP	A	16	37.446	50.118	23.529	1.00	11.17	6
ATOM	134	CB	ASP	A	16	36.924	50.059	22.068	1.00	11.99	6
ATOM	135	CG	ASP	A	16	35.761	49.101	21.873	1.00	12.89	6
ATOM	136	OD1	ASP	A	16	35.313	48.341	22.772	1.00	11.83	8
ATOM	137	OD2	ASP	A	16	35.244	49.114	20.732	1.00	14.31	8
ATOM	138	C	ASP	A	16	36.352	50.518	24.498	1.00	11.03	6
ATOM	139	O	ASP	A	16	35.768	51.582	24.289	1.00	11.12	8
ATOM	140	N	GLY	A	17	36.013	49.732	25.513	1.00	10.89	7
ATOM	141	CA	GLY	A	17	34.972	50.083	26.479	1.00	10.61	6
ATOM	142	C	GLY	A	17	33.545	50.032	25.938	1.00	10.65	6
ATOM	143	O	GLY	A	17	32.629	50.522	26.601	1.00	10.67	8
ATOM	144	N	GLN	A	18	33.287	49.436	24.766	1.00	10.50	7
ATOM	145	CA	GLN	A	18	31.995	49.346	24.151	1.00	10.55	6
ATOM	146	CB	GLN	A	18	32.064	49.835	22.691	1.00	15.25	6
ATOM	147	CG	GLN	A	18	32.718	51.182	22.436	1.00	21.24	6
ATOM	148	CD	GLN	A	18	31.729	52.313	22.693	1.00	25.84	6
ATOM	149	OE1	GLN	A	18	30.674	52.415	22.016	1.00	29.22	8
ATOM	150	NE2	GLN	A	18	32.104	53.124	23.668	1.00	27.29	7
ATOM	151	C	GLN	A	18	31.421	47.936	24.042	1.00	10.04	6
ATOM	152	O	GLN	A	18	30.467	47.808	23.281	1.00	9.96	8
ATOM	153	N	HIS	A	19	31.986	46.944	24.702	1.00	9.66	7
ATOM	154	CA	HIS	A	19	31.440	45.572	24.582	1.00	9.29	6
ATOM	155	CB	HIS	A	19	32.412	44.535	25.162	1.00	6.70	6
ATOM	156	CG	HIS	A	19	32.091	43.173	24.563	1.00	8.79	6
ATOM	157	CD2	HIS	A	19	31.749	41.987	25.138	1.00	7.93	6
ATOM	158	ND1	HIS	A	19	32.116	42.955	23.187	1.00	8.36	7
ATOM	159	CE1	HIS	A	19	31.825	41.705	22.909	1.00	8.32	6
ATOM	160	NE2	HIS	A	19	31.584	41.112	24.073	1.00	9.42	7
ATOM	161	C	HIS	A	19	30.007	45.489	25.132	1.00	9.04	6
ATOM	162	O	HIS	A	19	29.153	44.838	24.493	1.00	8.75	8
ATOM	163	N	TRP	A	20	29.650	46.184	26.217	1.00	9.17	7
ATOM	164	CA	TRP	A	20	28.248	46.090	26.688	1.00	9.56	6
ATOM	165	CB	TRP	A	20	28.200	46.691	28.093	1.00	8.24	6
ATOM	166	CG	TRP	A	20	29.112	46.119	29.122	1.00	7.50	6
ATOM	167	CD2	TRP	A	20	29.515	44.774	29.341	1.00	7.46	6
ATOM	168	CE2	TRP	A	20	30.374	44.751	30.459	1.00	7.35	6
ATOM	169	CE3	TRP	A	20	29.187	43.568	28.695	1.00	8.23	6
ATOM	170	CD1	TRP	A	20	29.736	46.854	30.088	1.00	7.37	6
ATOM	171	NE1	TRP	A	20	30.483	46.041	30.920	1.00	7.58	7
ATOM	172	CZ2	TRP	A	20	30.926	43.591	31.006	1.00	6.78	6
ATOM	173	CZ3	TRP	A	20	29.750	42.407	29.223	1.00	9.26	6
ATOM	174	CH2	TRP	A	20	30.608	42.427	30.366	1.00	7.69	6
ATOM	175	C	TRP	A	20	27.227	46.746	25.757	1.00	9.73	6
ATOM	176	O	TRP	A	20	26.070	46.395	25.592	1.00	9.42	8
ATOM	177	N	LYS	A	21	27.591	47.832	25.102	1.00	10.37	7
ATOM	178	CA	LYS	A	21	26.731	48.544	24.144	1.00	11.41	6
ATOM	179	CB	LYS	A	21	27.348	49.856	23.671	1.00	15.11	6
ATOM	180	CG	LYS	A	21	27.086	50.981	24.674	1.00	21.25	6
ATOM	181	CD	LYS	A	21	28.020	52.128	24.411	1.00	25.92	6
ATOM	182	CE	LYS	A	21	27.600	53.426	25.067	1.00	30.86	6
ATOM	183	NZ	LYS	A	21	27.119	54.448	24.030	1.00	34.41	7
ATOM	184	C	LYS	A	21	26.551	47.632	22.934	1.00	11.59	6
ATOM	185	O	LYS	A	21	25.474	47.562	22.400	1.00	11.80	8
ATOM	186	N	ARG	A	22	27.626	46.953	22.545	1.00	11.87	7
ATOM	187	CA	ARG	A	22	27.576	46.015	21.451	1.00	12.42	6
ATOM	188	CB	ARG	A	22	28.940	45.391	21.199	1.00	12.84	6
ATOM	189	CG	ARG	A	22	29.804	46.215	20.240	1.00	13.26	6
ATOM	190	CD	ARG	A	22	31.043	45.363	19.942	1.00	14.67	6
ATOM	191	NE	ARG	A	22	32.084	45.253	20.955	1.00	14.04	7
ATOM	192	CZ	ARG	A	22	33.068	46.161	21.065	1.00	14.66	6
ATOM	193	NH1	ARG	A	22	33.913	45.855	22.063	1.00	13.42	7
ATOM	194	NH2	ARG	A	22	33.206	47.242	20.261	1.00	12.34	7
ATOM	195	C	ARG	A	22	26.586	44.921	21.812	1.00	12.77	6
ATOM	196	O	ARG	A	22	25.682	44.543	21.038	1.00	13.11	8
ATOM	197	N	LEU	A	23	26.678	44.342	23.002	1.00	12.84	7
ATOM	198	CA	LEU	A	23	25.698	43.292	23.370	1.00	12.86	6
ATOM	199	CB	LEU	A	23	26.092	42.716	24.721	1.00	10.68	6
ATOM	200	CG	LEU	A	23	25.126	41.739	25.361	1.00	10.16	6
ATOM	201	CD1	LEU	A	23	24.804	40.562	24.449	1.00	8.43	6
ATOM	202	CD2	LEU	A	23	25.769	41.258	26.669	1.00	9.16	6
ATOM	203	C	LEU	A	23	24.285	43.874	23.388	1.00	13.25	6
ATOM	204	O	LEU	A	23	23.302	43.247	22.969	1.00	12.84	8
ATOM	205	N	GLN	A	24	24.144	45.123	23.873	1.00	13.66	7
ATOM	206	CA	GLN	A	24	22.848	45.781	23.929	1.00	14.44	6
ATOM	207	CB	GLN	A	24	22.959	47.205	24.523	1.00	16.30	6
ATOM	208	CG	GLN	A	24	21.578	47.851	24.620	1.00	18.17	6
ATOM	209	CD	GLN	A	24	21.659	49.208	25.296	1.00	20.30	6
ATOM	210	OE1	GLN	A	24	22.651	49.936	25.205	1.00	21.20	8
ATOM	211	NE2	GLN	A	24	20.619	49.539	26.023	1.00	20.53	7
ATOM	212	C	GLN	A	24	22.208	45.914	22.528	1.00	14.70	6

ATOM	213	O	GLN	A	24	21.030	45.626	22.296	1.00	14.63	8
ATOM	214	N	ASN	A	25	23.034	46.369	21.594	1.00	14.90	7
ATOM	215	CA	ASN	A	25	22.642	46.525	20.213	1.00	15.31	6
ATOM	216	CB	ASN	A	25	23.645	47.256	19.304	1.00	18.01	6
ATOM	217	CG	ASN	A	25	23.711	48.719	19.680	1.00	22.28	6
ATOM	218	OD1	ASN	A	25	22.686	49.238	20.127	1.00	24.44	8
ATOM	219	ND2	ASN	A	25	24.836	49.432	19.588	1.00	23.11	7
ATOM	220	C	ASN	A	25	22.371	45.141	19.588	1.00	15.19	6
ATOM	221	O	ASN	A	25	21.542	45.198	18.637	1.00	15.31	8
ATOM	222	N	ASP	A	26	22.954	44.059	20.051	1.00	14.67	7
ATOM	223	CA	ASP	A	26	22.647	42.765	19.394	1.00	14.48	6
ATOM	224	CB	ASP	A	26	24.002	42.002	19.440	1.00	14.63	6
ATOM	225	CG	ASP	A	26	24.340	41.059	18.322	1.00	14.74	6
ATOM	226	OD1	ASP	A	26	23.651	41.073	17.292	1.00	14.77	8
ATOM	227	OD2	ASP	A	26	25.294	40.238	18.363	1.00	14.65	8
ATOM	228	C	ASP	A	26	21.497	41.933	19.949	1.00	14.18	6
ATOM	229	O	ASP	A	26	21.119	40.869	19.454	1.00	13.76	8
ATOM	230	N	ALA	A	27	20.813	42.356	20.986	1.00	14.32	7
ATOM	231	CA	ALA	A	27	19.761	41.641	21.661	1.00	14.78	6
ATOM	232	CB	ALA	A	27	19.276	42.463	22.849	1.00	12.97	6
ATOM	233	C	ALA	A	27	18.627	41.207	20.754	1.00	15.34	6
ATOM	234	O	ALA	A	27	18.231	40.028	20.840	1.00	15.56	8
ATOM	235	N	GLU	A	28	18.099	42.032	19.858	1.00	15.76	7
ATOM	236	CA	GLU	A	28	17.010	41.598	18.984	1.00	16.05	6
ATOM	237	CB	GLU	A	28	16.526	42.815	18.170	1.00	23.00	6
ATOM	238	CG	GLU	A	28	15.097	42.736	17.596	1.00	31.01	6
ATOM	239	CD	GLU	A	28	14.001	42.258	18.547	1.00	36.48	6
ATOM	240	OE1	GLU	A	28	13.644	41.013	18.587	1.00	40.16	8
ATOM	241	OE2	GLU	A	28	13.427	43.089	19.316	1.00	38.33	8
ATOM	242	C	GLU	A	28	17.410	40.467	18.044	1.00	15.55	6
ATOM	243	O	GLU	A	28	16.773	39.435	17.835	1.00	15.27	8
ATOM	244	N	HIS	A	29	18.577	40.712	17.415	1.00	15.36	7
ATOM	245	CA	HIS	A	29	19.158	39.769	16.461	1.00	15.11	6
ATOM	246	CB	HIS	A	29	20.492	40.422	16.008	1.00	16.22	6
ATOM	247	CG	HIS	A	29	21.296	39.400	15.259	1.00	18.29	6
ATOM	248	CD2	HIS	A	29	20.895	38.501	14.294	1.00	18.16	6
ATOM	249	ND1	HIS	A	29	22.639	39.155	15.496	1.00	18.52	7
ATOM	250	CE1	HIS	A	29	23.055	38.163	14.693	1.00	18.61	6
ATOM	251	NE2	HIS	A	29	22.006	37.741	13.984	1.00	18.61	7
ATOM	252	C	HIS	A	29	19.282	38.370	17.059	1.00	14.84	6
ATOM	253	O	HIS	A	29	18.852	37.340	16.543	1.00	14.68	8
ATOM	254	N	LEU	A	30	19.913	38.292	18.233	1.00	14.66	7
ATOM	255	CA	LEU	A	30	20.154	37.107	19.020	1.00	14.56	6
ATOM	256	CB	LEU	A	30	20.913	37.409	20.319	1.00	13.60	6
ATOM	257	CG	LEU	A	30	22.350	37.884	20.194	1.00	15.00	6
ATOM	258	CD1	LEU	A	30	23.018	37.967	21.586	1.00	15.90	6
ATOM	259	CD2	LEU	A	30	23.229	37.049	19.292	1.00	14.94	6
ATOM	260	C	LEU	A	30	18.833	36.434	19.390	1.00	14.68	6
ATOM	261	O	LEU	A	30	18.683	35.228	19.248	1.00	14.21	8
ATOM	262	N	SER	A	31	17.877	37.240	19.879	1.00	15.37	7
ATOM	263	CA	SER	A	31	16.596	36.559	20.204	1.00	16.15	6
ATOM	264	CB	SER	A	31	15.603	37.378	21.005	1.00	17.82	6
ATOM	265	OG	SER	A	31	15.358	38.528	20.190	1.00	22.98	8
ATOM	266	C	SER	A	31	15.995	36.112	18.852	1.00	16.34	6
ATOM	267	O	SER	A	31	15.558	34.966	18.878	1.00	16.30	8
ATOM	268	N	ASP	A	32	16.021	36.882	17.765	1.00	16.40	7
ATOM	269	CA	ASP	A	32	15.477	36.341	16.518	1.00	16.55	6
ATOM	270	CB	ASP	A	32	15.485	37.339	15.370	1.00	22.70	6
ATOM	271	CG	ASP	A	32	14.756	38.665	15.583	1.00	27.13	6
ATOM	272	OD1	ASP	A	32	13.849	38.871	16.443	1.00	29.59	8
ATOM	273	OD2	ASP	A	32	15.122	39.661	14.868	1.00	29.28	8
ATOM	274	C	ASP	A	32	16.207	35.103	16.032	1.00	16.39	6
ATOM	275	O	ASP	A	32	15.416	34.249	15.583	1.00	16.54	8
ATOM	276	N	ILE	A	33	17.519	34.862	16.111	1.00	15.83	7
ATOM	277	CA	ILE	A	33	18.093	33.612	15.639	1.00	15.16	6
ATOM	278	CB	ILE	A	33	19.570	33.804	15.292	1.00	13.80	6
ATOM	279	CG2	ILE	A	33	19.681	34.906	14.219	1.00	11.75	6
ATOM	280	CG1	ILE	A	33	20.353	34.167	16.549	1.00	13.86	6
ATOM	281	CD1	ILE	A	33	21.822	34.372	16.151	1.00	14.13	6
ATOM	282	C	ILE	A	33	17.939	32.408	16.568	1.00	15.00	6
ATOM	283	O	ILE	A	33	18.342	31.264	16.207	1.00	15.20	8
ATOM	284	N	GLY	A	34	17.303	32.527	17.740	1.00	14.35	7
ATOM	285	CA	GLY	A	34	17.113	31.380	18.606	1.00	13.52	6
ATOM	286	C	GLY	A	34	18.042	31.270	19.790	1.00	12.87	6
ATOM	287	O	GLY	A	34	18.034	30.216	20.453	1.00	12.97	8
ATOM	288	N	ILE	A	35	18.796	32.320	20.120	1.00	12.23	7
ATOM	289	CA	ILE	A	35	19.679	32.268	21.301	1.00	11.16	6
ATOM	290	CB	ILE	A	35	20.812	33.277	21.168	1.00	9.65	6
ATOM	291	CG2	ILE	A	35	21.595	33.376	22.527	1.00	8.10	6
ATOM	292	CG1	ILE	A	35	21.782	33.025	20.002	1.00	9.07	6
ATOM	293	CD1	ILE	A	35	22.447	31.654	19.909	1.00	8.99	6
ATOM	294	C	ILE	A	35	18.798	32.522	22.516	1.00	10.71	6
ATOM	295	O	ILE	A	35	18.050	33.521	22.584	1.00	10.65	8
ATOM	296	N	THR	A	36	18.816	31.638	23.519	1.00	10.23	7
ATOM	297	CA	THR	A	36	18.010	31.768	24.713	1.00	9.85	6
ATOM	298	CB	THR	A	36	17.144	30.482	24.943	1.00	7.65	6
ATOM	299	OG1	THR	A	36	18.091	29.405	25.089	1.00	7.88	8
ATOM	300	CG2	THR	A	36	16.198	30.293	23.779	1.00	6.33	6
ATOM	301	C	THR	A	36	18.844	32.120	25.955	1.00	9.79	6
ATOM	302	O	THR	A	36	18.271	32.449	26.995	1.00	9.82	8
ATOM	303	N	ALA	A	37	20.160	32.045	25.937	1.00	9.41	7
ATOM	304	CA	ALA	A	37	20.970	32.392	27.086	1.00	9.45	6
ATOM	305	CB	ALA	A	37	21.169	31.279	28.113	1.00	5.60	6
ATOM	306	C	ALA	A	37	22.309	32.897	26.536	1.00	9.43	6
ATOM	307	O	ALA	A	37	22.815	32.383	25.562	1.00	9.36	8
ATOM	308	N	VAL	A	38	22.871	33.921	27.171	1.00	9.63	7
ATOM	309	CA	VAL	A	38	24.164	34.496	26.851	1.00	9.68	6
ATOM	310	CB	VAL	A	38	24.047	35.995	26.455	1.00	12.81	6
ATOM	311	CG1	VAL	A	38	25.397	36.673	26.290	1.00	14.06	6
ATOM	312	CG2	VAL	A	38	23.287	36.191	25.123	1.00	12.91	6
ATOM	313	C	VAL	A	38	25.124	34.326	28.042	1.00	9.49	6
ATOM	314	O	VAL	A	38	24.720	34.563	29.197	1.00	9.44	8
ATOM	315	N	TRP	A	39	26.371	33.915	27.799	1.00	9.06	7
ATOM	316	CA	TRP	A	39	27.447	33.825	28.774	1.00	8.66	6
ATOM	317	CB	TRP	A	39	28.188	32.492	28.797	1.00	7.03	6
ATOM	318	CG	TRP	A	39	29.612	32.554	29.282	1.00	6.23	6

ATOM	319	CD2	TRP	A	39	30.691	31.682	28.807	1.00	6.00	6
ATOM	320	CE2	TRP	A	39	31.875	32.074	29.473	1.00	5.58	6
ATOM	321	CE3	TRP	A	39	30.708	30.585	27.908	1.00	5.00	6
ATOM	322	CD1	TRP	A	39	30.201	33.372	30.190	1.00	5.74	6
ATOM	323	NE1	TRP	A	39	31.568	33.153	30.268	1.00	5.57	7
ATOM	324	CZ2	TRP	A	39	33.099	31.441	29.211	1.00	5.00	6
ATOM	325	CZ3	TRP	A	39	31.955	29.964	27.701	1.00	5.00	6
ATOM	326	CH2	TRP	A	39	33.115	30.400	28.307	1.00	5.00	6
ATOM	327	C	TRP	A	39	28.317	35.078	28.452	1.00	8.53	6
ATOM	328	O	TRP	A	39	28.856	35.399	27.384	1.00	8.32	8
ATOM	329	N	ILE	A	40	28.431	35.945	29.459	1.00	8.37	7
ATOM	330	CA	ILE	A	40	29.143	37.247	29.467	1.00	8.51	6
ATOM	331	CB	ILE	A	40	28.091	38.113	30.259	1.00	9.85	6
ATOM	332	CG2	ILE	A	40	28.089	38.802	31.613	1.00	9.64	6
ATOM	333	CG1	ILE	A	40	27.803	39.287	29.286	1.00	9.52	6
ATOM	334	CD1	ILE	A	40	26.594	38.637	28.616	1.00	11.76	6
ATOM	335	C	ILE	A	40	30.524	37.121	30.063	1.00	8.39	6
ATOM	336	O	ILE	A	40	30.680	36.373	31.033	1.00	8.04	8
ATOM	337	N	PRO	A	41	31.571	37.800	29.564	1.00	8.30	7
ATOM	338	CD	PRO	A	41	31.469	38.773	28.451	1.00	8.06	6
ATOM	339	CA	PRO	A	41	32.887	37.771	30.151	1.00	8.14	6
ATOM	340	CB	PRO	A	41	33.802	38.683	29.246	1.00	8.13	6
ATOM	341	CG	PRO	A	41	32.756	39.565	28.595	1.00	8.01	6
ATOM	342	C	PRO	A	41	32.846	38.312	31.590	1.00	7.87	6
ATOM	343	O	PRO	A	41	31.891	38.952	32.039	1.00	7.72	8
ATOM	344	N	PRO	A	42	33.909	38.044	32.341	1.00	7.64	7
ATOM	345	CD	PRO	A	42	35.113	37.297	31.880	1.00	7.36	6
ATOM	346	CA	PRO	A	42	34.084	38.542	33.711	1.00	7.41	6
ATOM	347	CB	PRO	A	42	35.490	38.085	34.191	1.00	7.45	6
ATOM	348	CG	PRO	A	42	35.772	36.947	33.217	1.00	7.45	6
ATOM	349	C	PRO	A	42	33.841	40.054	33.685	1.00	7.06	6
ATOM	350	O	PRO	A	42	34.481	40.819	32.931	1.00	6.95	8
ATOM	351	N	ALA	A	43	32.875	40.536	34.452	1.00	6.53	7
ATOM	352	CA	ALA	A	43	32.477	41.937	34.481	1.00	6.39	6
ATOM	353	CB	ALA	A	43	30.968	41.991	34.756	1.00	5.00	6
ATOM	354	C	ALA	A	43	33.131	42.845	35.529	1.00	6.36	6
ATOM	355	O	ALA	A	43	32.847	44.042	35.582	1.00	6.42	8
ATOM	356	N	TYR	A	44	33.995	42.333	36.394	1.00	6.22	7
ATOM	357	CA	TYR	A	44	34.637	43.052	37.465	1.00	6.10	6
ATOM	358	CB	TYR	A	44	34.455	42.266	38.819	1.00	6.31	6
ATOM	359	CG	TYR	A	44	34.381	40.781	38.551	1.00	6.51	6
ATOM	360	CD1	TYR	A	44	35.538	40.086	38.145	1.00	6.67	6
ATOM	361	CE1	TYR	A	44	35.472	38.732	37.848	1.00	6.66	6
ATOM	362	CD2	TYR	A	44	33.200	40.071	38.613	1.00	6.52	6
ATOM	363	CE2	TYR	A	44	33.108	38.722	38.301	1.00	6.55	6
ATOM	364	CZ	TYR	A	44	34.276	38.073	37.917	1.00	6.98	6
ATOM	365	OH	TYR	A	44	34.209	36.729	37.568	1.00	7.43	8
ATOM	366	C	TYR	A	44	36.060	43.413	37.075	1.00	5.99	6
ATOM	367	O	TYR	A	44	36.682	42.945	36.097	1.00	5.98	8
ATOM	368	N	LYS	A	45	36.556	44.410	37.815	1.00	5.93	7
ATOM	369	CA	LYS	A	45	37.865	45.003	37.587	1.00	5.73	6
ATOM	370	CB	LYS	A	45	38.033	46.160	38.580	1.00	5.00	6
ATOM	371	CG	LYS	A	45	39.192	47.127	38.251	1.00	5.00	6
ATOM	372	CD	LYS	A	45	39.093	48.021	37.024	1.00	5.00	6
ATOM	373	CE	LYS	A	45	37.830	48.865	36.976	1.00	5.00	6
ATOM	374	NZ	LYS	A	45	37.599	49.990	37.908	1.00	5.00	7
ATOM	375	C	LYS	A	45	39.029	44.010	37.657	1.00	5.87	6
ATOM	376	O	LYS	A	45	39.207	43.306	38.636	1.00	5.70	8
ATOM	377	N	GLY	A	46	39.847	43.978	36.608	1.00	6.09	7
ATOM	378	CA	GLY	A	46	41.017	43.149	36.478	1.00	6.70	6
ATOM	379	C	GLY	A	46	42.246	43.917	36.957	1.00	7.41	6
ATOM	380	O	GLY	A	46	42.171	45.098	37.382	1.00	7.54	8
ATOM	381	N	LEU	A	47	43.420	43.291	36.970	1.00	7.77	7
ATOM	382	CA	LEU	A	47	44.681	43.889	37.385	1.00	8.34	6
ATOM	383	CB	LEU	A	47	45.838	42.922	37.455	1.00	9.18	6
ATOM	384	CG	LEU	A	47	46.426	42.140	36.297	1.00	11.32	6
ATOM	385	CD1	LEU	A	47	45.419	41.207	35.660	1.00	12.40	6
ATOM	386	CD2	LEU	A	47	46.897	42.995	35.137	1.00	12.34	6
ATOM	387	C	LEU	A	47	45.040	45.105	36.483	1.00	8.70	6
ATOM	388	O	LEU	A	47	45.884	45.929	36.872	1.00	8.67	8
ATOM	389	N	SER	A	48	44.451	45.283	35.303	1.00	8.86	7
ATOM	390	CA	SER	A	48	44.667	46.453	34.457	1.00	9.11	6
ATOM	391	CB	SER	A	48	45.870	46.312	33.492	1.00	9.17	6
ATOM	392	OG	SER	A	48	45.546	45.387	32.490	1.00	8.88	8
ATOM	393	C	SER	A	48	43.380	46.678	33.672	1.00	9.13	6
ATOM	394	O	SER	A	48	42.533	45.777	33.610	1.00	9.05	8
ATOM	395	N	GLN	A	49	43.225	47.807	33.003	1.00	9.23	7
ATOM	396	CA	GLN	A	49	42.076	48.113	32.174	1.00	9.17	6
ATOM	397	CB	GLN	A	49	42.104	49.549	31.592	1.00	6.81	6
ATOM	398	CG	GLN	A	49	40.813	49.921	30.864	1.00	5.86	6
ATOM	399	CD	GLN	A	49	41.078	51.178	30.041	1.00	7.48	6
ATOM	400	OE1	GLN	A	49	41.898	51.153	29.103	1.00	7.62	8
ATOM	401	NE2	GLN	A	49	40.489	52.278	30.467	1.00	5.00	7
ATOM	402	C	GLN	A	49	41.929	47.121	31.006	1.00	9.30	6
ATOM	403	O	GLN	A	49	40.774	46.745	30.647	1.00	9.52	8
ATOM	404	N	SER	A	50	43.038	46.690	30.424	1.00	9.20	7
ATOM	405	CA	SER	A	50	42.992	45.763	29.281	1.00	9.33	6
ATOM	406	CB	SER	A	50	44.173	46.116	28.346	1.00	11.13	6
ATOM	407	OG	SER	A	50	45.417	45.891	29.000	1.00	14.96	8
ATOM	408	C	SER	A	50	42.924	44.272	29.626	1.00	8.88	6
ATOM	409	O	SER	A	50	42.810	43.409	28.736	1.00	8.96	8
ATOM	410	N	ASP	A	51	42.910	43.891	30.881	1.00	8.41	7
ATOM	411	CA	ASP	A	51	42.812	42.467	31.211	1.00	7.98	6
ATOM	412	CB	ASP	A	51	43.030	42.303	32.724	1.00	7.44	6
ATOM	413	CG	ASP	A	51	43.044	40.822	33.120	1.00	8.58	6
ATOM	414	OD1	ASP	A	51	44.069	40.115	32.869	1.00	8.63	8
ATOM	415	OD2	ASP	A	51	41.992	40.399	33.679	1.00	8.06	8
ATOM	416	C	ASP	A	51	41.460	41.932	30.766	1.00	7.80	6
ATOM	417	O	ASP	A	51	40.441	42.613	30.990	1.00	7.70	8
ATOM	418	N	ASN	A	52	41.330	40.729	30.217	1.00	7.56	7
ATOM	419	CA	ASN	A	52	40.040	40.182	29.867	1.00	7.47	6
ATOM	420	CB	ASN	A	52	40.175	38.887	29.057	1.00	9.45	6
ATOM	421	CG	ASN	A	52	40.562	39.187	27.620	1.00	12.85	6
ATOM	422	OD1	ASN	A	52	40.516	40.341	27.167	1.00	15.76	8
ATOM	423	ND2	ASN	A	52	40.979	38.239	26.786	1.00	12.70	7
ATOM	424	C	ASN	A	52	39.166	39.829	31.071	1.00	7.16	6

ATOM	425	O	ASN	A	52	38.007	39.399	30.782	1.00	7.11	8
ATOM	426	N	GLY	A	53	39.652	39.949	32.309	1.00	6.67	7
ATOM	427	CA	GLY	A	53	38.832	39.609	33.457	1.00	6.52	6
ATOM	428	C	GLY	A	53	39.262	38.324	34.124	1.00	6.62	6
ATOM	429	O	GLY	A	53	38.726	38.021	35.199	1.00	6.84	8
ATOM	430	N	TYR	A	54	40.227	37.565	33.548	1.00	6.28	7
ATOM	431	CA	TYR	A	54	40.722	36.331	34.179	1.00	5.98	6
ATOM	432	CB	TYR	A	54	41.027	35.227	33.116	1.00	6.06	6
ATOM	433	CG	TYR	A	54	39.720	34.834	32.427	1.00	5.99	6
ATOM	434	CD1	TYR	A	54	39.481	35.232	31.108	1.00	6.44	6
ATOM	435	CE1	TYR	A	54	38.251	34.920	30.492	1.00	6.68	6
ATOM	436	CD2	TYR	A	54	38.700	34.194	33.088	1.00	5.97	6
ATOM	437	CE2	TYR	A	54	37.474	33.857	32.517	1.00	6.05	6
ATOM	438	CZ	TYR	A	54	37.282	34.209	31.182	1.00	6.50	6
ATOM	439	OH	TYR	A	54	36.083	33.928	30.558	1.00	6.69	8
ATOM	440	C	TYR	A	54	41.879	36.549	35.145	1.00	5.76	6
ATOM	441	O	TYR	A	54	42.441	35.655	35.818	1.00	5.63	8
ATOM	442	N	GLY	A	55	42.237	37.799	35.429	1.00	5.53	7
ATOM	443	CA	GLY	A	55	43.226	38.205	36.438	1.00	5.64	6
ATOM	444	C	GLY	A	55	42.464	39.315	37.256	1.00	5.59	6
ATOM	445	O	GLY	A	55	42.818	40.499	37.213	1.00	5.60	8
ATOM	446	N	PRO	A	56	41.410	38.876	37.948	1.00	5.20	7
ATOM	447	CD	PRO	A	56	40.952	37.502	38.113	1.00	5.03	6
ATOM	448	CA	PRO	A	56	40.567	39.757	38.732	1.00	5.12	6
ATOM	449	CB	PRO	A	56	39.282	38.948	39.083	1.00	5.13	6
ATOM	450	CG	PRO	A	56	39.914	37.555	39.212	1.00	5.03	6
ATOM	451	C	PRO	A	56	41.189	40.335	39.998	1.00	5.03	6
ATOM	452	O	PRO	A	56	41.728	39.671	40.862	1.00	5.00	8
ATOM	453	N	TYR	A	57	41.081	41.640	40.099	1.00	5.00	7
ATOM	454	CA	TYR	A	57	41.499	42.474	41.207	1.00	5.00	6
ATOM	455	CB	TYR	A	57	42.042	43.842	40.709	1.00	5.45	6
ATOM	456	CG	TYR	A	57	42.261	44.833	41.840	1.00	6.29	6
ATOM	457	CD1	TYR	A	57	43.330	44.634	42.730	1.00	6.86	6
ATOM	458	CE1	TYR	A	57	43.521	45.499	43.810	1.00	7.20	6
ATOM	459	CD2	TYR	A	57	41.421	45.913	42.014	1.00	6.52	6
ATOM	460	CE2	TYR	A	57	41.634	46.788	43.085	1.00	6.96	6
ATOM	461	CZ	TYR	A	57	42.669	46.566	43.963	1.00	7.37	6
ATOM	462	OH	TYR	A	57	42.835	47.431	45.036	1.00	7.85	8
ATOM	463	C	TYR	A	57	40.372	42.683	42.201	1.00	5.00	6
ATOM	464	O	TYR	A	57	40.546	42.347	43.362	1.00	5.00	8
ATOM	465	N	ASP	A	58	39.210	43.212	41.826	1.00	5.00	7
ATOM	466	CA	ASP	A	58	38.134	43.465	42.771	1.00	5.00	6
ATOM	467	CB	ASP	A	58	38.136	44.990	43.088	1.00	5.00	6
ATOM	468	CG	ASP	A	58	37.210	45.478	44.152	1.00	5.00	6
ATOM	469	OD1	ASP	A	58	36.550	44.681	44.829	1.00	5.00	8
ATOM	470	OD2	ASP	A	58	36.995	46.702	44.348	1.00	5.00	8
ATOM	471	C	ASP	A	58	36.813	42.974	42.250	1.00	5.00	6
ATOM	472	O	ASP	A	58	36.226	43.643	41.379	1.00	5.00	8
ATOM	473	N	LEU	A	59	36.258	41.917	42.874	1.00	5.00	7
ATOM	474	CA	LEU	A	59	34.967	41.399	42.426	1.00	5.00	6
ATOM	475	CB	LEU	A	59	34.696	40.040	43.128	1.00	6.31	6
ATOM	476	CG	LEU	A	59	35.782	38.942	42.885	1.00	8.19	6
ATOM	477	CD1	LEU	A	59	35.479	37.701	43.725	1.00	7.46	6
ATOM	478	CD2	LEU	A	59	35.960	38.571	41.423	1.00	6.96	6
ATOM	479	C	LEU	A	59	33.758	42.311	42.650	1.00	5.05	6
ATOM	480	O	LEU	A	59	32.644	42.112	42.100	1.00	5.00	8
ATOM	481	N	TYR	A	60	33.921	43.352	43.480	1.00	5.25	7
ATOM	482	CA	TYR	A	60	32.804	44.266	43.786	1.00	5.52	6
ATOM	483	CB	TYR	A	60	32.811	44.611	45.271	1.00	5.24	6
ATOM	484	CG	TYR	A	60	32.214	43.597	46.224	1.00	5.38	6
ATOM	485	CD1	TYR	A	60	33.101	42.761	46.929	1.00	5.65	6
ATOM	486	CE1	TYR	A	60	32.646	41.833	47.866	1.00	5.89	6
ATOM	487	CD2	TYR	A	60	30.855	43.441	46.441	1.00	5.22	6
ATOM	488	CE2	TYR	A	60	30.359	42.520	47.333	1.00	5.60	6
ATOM	489	CZ	TYR	A	60	31.255	41.742	48.063	1.00	6.27	6
ATOM	490	OH	TYR	A	60	30.867	40.764	48.957	1.00	6.71	8
ATOM	491	C	TYR	A	60	32.888	45.540	42.937	1.00	5.77	6
ATOM	492	O	TYR	A	60	32.117	46.467	43.158	1.00	6.16	8
ATOM	493	N	ASP	A	61	33.824	45.690	42.052	1.00	5.53	7
ATOM	494	CA	ASP	A	61	33.963	46.831	41.196	1.00	5.82	6
ATOM	495	CB	ASP	A	61	35.395	47.325	41.096	1.00	5.00	6
ATOM	496	CG	ASP	A	61	35.635	48.569	40.256	1.00	5.28	6
ATOM	497	OD1	ASP	A	61	34.717	49.013	39.468	1.00	6.54	8
ATOM	498	OD2	ASP	A	61	36.778	49.132	40.283	1.00	5.00	8
ATOM	499	C	ASP	A	61	33.455	46.390	39.790	1.00	6.20	6
ATOM	500	O	ASP	A	61	34.313	45.844	39.065	1.00	6.25	8
ATOM	501	N	LEU	A	62	32.228	46.606	39.374	1.00	6.27	7
ATOM	502	CA	LEU	A	62	31.732	46.208	38.072	1.00	6.89	6
ATOM	503	CB	LEU	A	62	30.242	45.815	38.193	1.00	7.43	6
ATOM	504	CG	LEU	A	62	29.864	44.704	39.231	1.00	9.12	6
ATOM	505	CD1	LEU	A	62	28.372	44.443	39.402	1.00	6.08	6
ATOM	506	CD2	LEU	A	62	30.514	43.357	38.889	1.00	9.37	6
ATOM	507	C	LEU	A	62	31.934	47.317	37.053	1.00	7.56	6
ATOM	508	O	LEU	A	62	31.256	47.422	36.044	1.00	7.76	8
ATOM	509	N	GLY	A	63	32.908	48.240	37.209	1.00	7.95	7
ATOM	510	CA	GLY	A	63	33.125	49.350	36.307	1.00	7.98	6
ATOM	511	C	GLY	A	63	32.529	50.656	36.862	1.00	8.19	6
ATOM	512	O	GLY	A	63	31.954	51.380	36.064	1.00	7.99	8
ATOM	513	N	GLU	A	64	32.685	50.974	38.143	1.00	8.78	7
ATOM	514	CA	GLU	A	64	32.154	52.244	38.659	1.00	9.55	6
ATOM	515	CB	GLU	A	64	30.831	52.051	39.398	1.00	10.66	6
ATOM	516	CG	GLU	A	64	30.916	51.052	40.517	1.00	11.34	6
ATOM	517	CD	GLU	A	64	29.629	50.986	41.287	1.00	13.83	6
ATOM	518	OE1	GLU	A	64	29.203	49.959	41.856	1.00	16.12	8
ATOM	519	OE2	GLU	A	64	28.864	51.950	41.397	1.00	15.85	8
ATOM	520	C	GLU	A	64	33.046	52.958	39.664	1.00	9.91	6
ATOM	521	O	GLU	A	64	32.691	53.987	40.243	1.00	9.88	8
ATOM	522	N	PHE	A	65	34.212	52.363	39.936	1.00	10.20	7
ATOM	523	CA	PHE	A	65	35.172	52.891	40.884	1.00	10.39	6
ATOM	524	CB	PHE	A	65	35.412	51.981	42.114	1.00	9.02	6
ATOM	525	CG	PHE	A	65	34.151	51.662	42.878	1.00	8.75	6
ATOM	526	CD1	PHE	A	65	33.541	50.420	42.829	1.00	7.83	6
ATOM	527	CD2	PHE	A	65	33.508	52.662	43.617	1.00	7.65	6
ATOM	528	CE1	PHE	A	65	32.339	50.164	43.499	1.00	6.31	6
ATOM	529	CE2	PHE	A	65	32.322	52.406	44.296	1.00	6.18	6
ATOM	530	CZ	PHE	A	65	31.739	51.138	44.248	1.00	5.83	6

SUBSTITUTE SHEET (RULE 26)

Appendix 1

ATOM	531	C	PHE	A	65	36.480	53.123	40.126	1.00	10.75	6
ATOM	532	O	PHE	A	65	36.935	52.381	39.255	1.00	10.67	8
ATOM	533	N	GLN	A	66	37.091	54.215	40.584	1.00	11.02	7
ATOM	534	CA	GLN	A	66	38.370	54.590	39.964	1.00	11.57	6
ATOM	535	CB	GLN	A	66	38.512	56.102	40.168	1.00	15.18	6
ATOM	536	CG	GLN	A	66	39.855	56.661	39.832	1.00	20.59	6
ATOM	537	CD	GLN	A	66	40.150	56.793	38.363	1.00	24.82	6
ATOM	538	OE1	GLN	A	66	39.958	57.812	37.688	1.00	28.38	8
ATOM	539	NE2	GLN	A	66	40.716	55.789	37.719	1.00	26.84	7
ATOM	540	C	GLN	A	66	39.489	53.768	40.576	1.00	11.54	6
ATOM	541	O	GLN	A	66	39.989	54.089	41.699	1.00	11.29	8
ATOM	542	N	GLN	A	67	39.870	52.683	39.895	1.00	11.31	7
ATOM	543	CA	GLN	A	67	40.915	51.786	40.411	1.00	11.24	6
ATOM	544	CB	GLN	A	67	40.390	50.591	41.201	1.00	9.56	6
ATOM	545	CG	GLN	A	67	39.353	50.740	42.242	1.00	7.94	6
ATOM	546	CD	GLN	A	67	38.970	49.695	43.240	1.00	6.97	6
ATOM	547	OE1	GLN	A	67	39.359	49.865	44.405	1.00	7.23	8
ATOM	548	NE2	GLN	A	67	38.222	48.659	42.932	1.00	5.00	7
ATOM	549	C	GLN	A	67	41.738	51.246	39.242	1.00	11.63	6
ATOM	550	O	GLN	A	67	41.158	50.867	38.216	1.00	11.46	8
ATOM	551	N	LYS	A	68	43.063	51.149	39.341	1.00	12.10	7
ATOM	552	CA	LYS	A	68	43.938	50.664	38.285	1.00	12.61	6
ATOM	553	CB	LYS	A	68	43.621	49.280	37.709	1.00	13.06	6
ATOM	554	CG	LYS	A	68	43.465	48.179	38.780	1.00	14.46	6
ATOM	555	CD	LYS	A	68	44.715	48.024	39.626	1.00	15.01	6
ATOM	556	CE	LYS	A	68	44.683	47.225	40.918	1.00	14.26	6
ATOM	557	NZ	LYS	A	68	46.062	47.066	41.499	1.00	12.89	7
ATOM	558	C	LYS	A	68	43.908	51.710	37.178	1.00	13.39	6
ATOM	559	O	LYS	A	68	43.978	51.422	35.955	1.00	14.41	8
ATOM	560	N	GLY	A	69	43.764	53.001	37.484	1.00	13.13	7
ATOM	561	CA	GLY	A	69	43.739	54.115	36.582	1.00	12.76	6
ATOM	562	C	GLY	A	69	42.535	54.177	35.674	1.00	12.59	6
ATOM	563	O	GLY	A	69	42.481	54.975	34.735	1.00	12.74	8
ATOM	564	N	THR	A	70	41.497	53.394	35.983	1.00	12.05	7
ATOM	565	CA	THR	A	70	40.325	53.375	35.120	1.00	11.09	6
ATOM	566	CB	THR	A	70	40.536	52.215	34.122	1.00	9.79	6
ATOM	567	OG1	THR	A	70	39.502	52.210	33.117	1.00	10.12	8
ATOM	568	CG2	THR	A	70	40.547	50.831	34.773	1.00	9.26	6
ATOM	569	C	THR	A	70	39.087	53.169	35.950	1.00	10.63	6
ATOM	570	O	THR	A	70	39.115	52.524	36.977	1.00	10.42	8
ATOM	571	N	VAL	A	71	37.978	53.737	35.484	1.00	10.18	7
ATOM	572	CA	VAL	A	71	36.690	53.549	36.107	1.00	9.77	6
ATOM	573	CB	VAL	A	71	35.802	54.788	35.985	1.00	10.20	6
ATOM	574	CG1	VAL	A	71	34.374	54.448	36.303	1.00	8.33	6
ATOM	575	CG2	VAL	A	71	36.393	55.860	36.919	1.00	9.35	6
ATOM	576	C	VAL	A	71	36.093	52.313	35.404	1.00	9.37	6
ATOM	577	O	VAL	A	71	35.766	51.299	36.050	1.00	9.39	8
ATOM	578	N	ARG	A	72	36.007	52.357	34.089	1.00	8.79	7
ATOM	579	CA	ARG	A	72	35.449	51.252	33.344	1.00	8.64	6
ATOM	580	CB	ARG	A	72	35.205	51.645	31.846	1.00	7.09	6
ATOM	581	CG	ARG	A	72	36.443	51.798	30.962	1.00	6.38	6
ATOM	582	CD	ARG	A	72	36.054	51.979	29.499	1.00	6.64	6
ATOM	583	NE	ARG	A	72	37.131	52.071	28.536	1.00	6.31	7
ATOM	584	CZ	ARG	A	72	38.053	51.266	28.054	1.00	5.00	6
ATOM	585	NH1	ARG	A	72	38.926	51.664	27.158	1.00	5.00	7
ATOM	586	NH2	ARG	A	72	38.043	50.022	28.506	1.00	5.00	7
ATOM	587	C	ARG	A	72	36.316	49.984	33.347	1.00	8.29	6
ATOM	588	O	ARG	A	72	37.531	50.080	33.499	1.00	8.41	8
ATOM	589	N	THR	A	73	35.700	48.836	33.120	1.00	8.00	7
ATOM	590	CA	THR	A	73	36.539	47.632	32.967	1.00	8.12	6
ATOM	591	CB	THR	A	73	35.820	46.301	33.270	1.00	6.10	6
ATOM	592	OG1	THR	A	73	34.727	46.140	32.317	1.00	5.35	8
ATOM	593	CG2	THR	A	73	35.361	46.223	34.730	1.00	5.00	6
ATOM	594	C	THR	A	73	36.932	47.628	31.481	1.00	8.12	6
ATOM	595	O	THR	A	73	36.630	48.581	30.739	1.00	8.16	8
ATOM	596	N	LYS	A	74	37.514	46.575	30.939	1.00	8.08	7
ATOM	597	CA	LYS	A	74	37.782	46.496	29.508	1.00	8.07	6
ATOM	598	CB	LYS	A	74	38.443	45.122	29.215	1.00	7.37	6
ATOM	599	CG	LYS	A	74	38.780	44.864	27.777	1.00	7.51	6
ATOM	600	CD	LYS	A	74	39.173	43.465	27.359	1.00	6.71	6
ATOM	601	CE	LYS	A	74	39.463	43.461	25.867	1.00	7.86	6
ATOM	602	NZ	LYS	A	74	40.043	42.121	25.465	1.00	7.32	7
ATOM	603	C	LYS	A	74	36.469	46.596	28.696	1.00	7.96	6
ATOM	604	O	LYS	A	74	36.376	47.163	27.598	1.00	7.92	8
ATOM	605	N	TYR	A	75	35.375	46.004	29.221	1.00	7.80	7
ATOM	606	CA	TYR	A	75	34.113	45.937	28.503	1.00	7.58	6
ATOM	607	CB	TYR	A	75	33.400	44.620	29.024	1.00	7.14	6
ATOM	608	CG	TYR	A	75	34.311	43.409	28.864	1.00	6.68	6
ATOM	609	CD1	TYR	A	75	34.853	42.777	29.988	1.00	6.37	6
ATOM	610	CE1	TYR	A	75	35.716	41.696	29.857	1.00	6.28	6
ATOM	611	CD2	TYR	A	75	34.677	42.916	27.589	1.00	6.45	6
ATOM	612	CE2	TYR	A	75	35.547	41.855	27.414	1.00	6.14	6
ATOM	613	CZ	TYR	A	75	36.039	41.257	28.570	1.00	6.25	6
ATOM	614	OH	TYR	A	75	36.913	40.195	28.479	1.00	6.33	8
ATOM	615	C	TYR	A	75	33.188	47.141	28.576	1.00	7.81	6
ATOM	616	O	TYR	A	75	32.274	47.302	27.713	1.00	7.79	8
ATOM	617	N	GLY	A	76	33.355	48.068	29.555	1.00	7.71	7
ATOM	618	CA	GLY	A	76	32.468	49.243	29.681	1.00	7.27	6
ATOM	619	C	GLY	A	76	32.204	49.486	31.152	1.00	7.13	6
ATOM	620	O	GLY	A	76	32.841	48.904	32.048	1.00	6.91	8
ATOM	621	N	THR	A	77	31.250	50.356	31.425	1.00	7.24	7
ATOM	622	CA	THR	A	77	30.855	50.694	32.813	1.00	7.52	6
ATOM	623	CB	THR	A	77	30.386	52.172	32.914	1.00	7.84	6
ATOM	624	OG1	THR	A	77	29.223	52.337	32.073	1.00	8.21	8
ATOM	625	CG2	THR	A	77	31.378	53.173	32.361	1.00	6.70	6
ATOM	626	C	THR	A	77	29.712	49.827	33.304	1.00	7.62	6
ATOM	627	O	THR	A	77	28.984	49.118	32.575	1.00	7.39	8
ATOM	628	N	LYS	A	78	29.460	49.853	34.611	1.00	7.89	7
ATOM	629	CA	LYS	A	78	28.398	49.084	35.247	1.00	8.24	6
ATOM	630	CB	LYS	A	78	28.465	49.384	36.759	1.00	8.87	6
ATOM	631	CG	LYS	A	78	27.449	48.604	37.551	1.00	11.52	6
ATOM	632	CD	LYS	A	78	27.592	49.117	39.004	1.00	13.82	6
ATOM	633	CE	LYS	A	78	26.681	48.228	39.824	1.00	15.45	6
ATOM	634	NZ	LYS	A	78	26.132	49.000	40.954	1.00	18.28	7
ATOM	635	C	LYS	A	78	27.022	49.428	34.735	1.00	8.73	6
ATOM	636	O	LYS	A	78	26.165	48.565	34.477	1.00	8.67	8

ATOM	637	N	SER	A	79	26.749	50.759	34.578	1.00	9.32	7
ATOM	638	CA	SER	A	79	25.401	51.141	34.086	1.00	9.71	6
ATOM	639	CB	SER	A	79	25.190	52.607	34.380	1.00	12.14	6
ATOM	640	OG	SER	A	79	25.960	53.338	33.488	1.00	15.84	8
ATOM	641	C	SER	A	79	25.262	50.703	32.644	1.00	9.79	6
ATOM	642	O	SER	A	79	24.142	50.254	32.312	1.00	10.15	8
ATOM	643	N	GLU	A	80	26.291	50.655	31.814	1.00	9.56	7
ATOM	644	CA	GLU	A	80	26.160	50.128	30.452	1.00	9.39	6
ATOM	645	CB	GLU	A	80	27.429	50.452	29.723	1.00	10.04	6
ATOM	646	CG	GLU	A	80	27.546	51.928	29.378	1.00	11.54	6
ATOM	647	CD	GLU	A	80	28.902	52.167	28.769	1.00	14.36	6
ATOM	648	OE1	GLU	A	80	29.881	51.408	28.913	1.00	15.28	8
ATOM	649	OE2	GLU	A	80	29.051	53.186	28.075	1.00	18.22	8
ATOM	650	C	GLU	A	80	25.853	48.629	30.476	1.00	9.05	6
ATOM	651	O	GLU	A	80	25.005	48.179	29.720	1.00	8.72	8
ATOM	652	N	LEU	A	81	26.441	47.873	31.394	1.00	9.09	7
ATOM	653	CA	LEU	A	81	26.145	46.428	31.534	1.00	9.12	6
ATOM	654	CB	LEU	A	81	27.188	45.716	32.385	1.00	8.24	6
ATOM	655	CG	LEU	A	81	26.866	44.272	32.843	1.00	8.68	6
ATOM	656	CD1	LEU	A	81	26.744	43.229	31.738	1.00	7.74	6
ATOM	657	CD2	LEU	A	81	27.983	43.841	33.771	1.00	9.60	6
ATOM	658	C	LEU	A	81	24.710	46.226	32.053	1.00	9.19	6
ATOM	659	O	LEU	A	81	23.952	45.386	31.515	1.00	8.94	8
ATOM	660	N	GLN	A	82	24.247	47.005	33.042	1.00	9.33	7
ATOM	661	CA	GLN	A	82	22.853	46.834	33.479	1.00	9.81	6
ATOM	662	CB	GLN	A	82	22.588	47.739	34.681	1.00	11.55	6
ATOM	663	CG	GLN	A	82	23.288	47.105	35.901	1.00	14.03	6
ATOM	664	CD	GLN	A	82	23.239	47.993	37.132	1.00	14.62	6
ATOM	665	OE1	GLN	A	82	23.497	49.180	36.990	1.00	15.76	8
ATOM	666	NE2	GLN	A	82	22.947	47.380	38.266	1.00	14.70	7
ATOM	667	C	GLN	A	82	21.878	47.108	32.358	1.00	10.18	6
ATOM	668	O	GLN	A	82	20.854	46.455	32.247	1.00	10.30	8
ATOM	669	N	ASP	A	83	22.106	48.088	31.501	1.00	10.58	7
ATOM	670	CA	ASP	A	83	21.281	48.355	30.317	1.00	11.05	6
ATOM	671	CB	ASP	A	83	21.631	49.619	29.514	1.00	15.09	6
ATOM	672	CG	ASP	A	83	21.228	50.893	30.246	1.00	18.79	6
ATOM	673	OD1	ASP	A	83	20.404	50.950	31.175	1.00	18.59	8
ATOM	674	OD2	ASP	A	83	21.832	51.914	29.841	1.00	22.13	8
ATOM	675	C	ASP	A	83	21.439	47.203	29.307	1.00	10.81	6
ATOM	676	O	ASP	A	83	20.391	46.942	28.751	1.00	11.02	8
ATOM	677	N	ALA	A	84	22.562	46.574	29.048	1.00	10.37	7
ATOM	678	CA	ALA	A	84	22.630	45.461	28.120	1.00	10.32	6
ATOM	679	CB	ALA	A	84	24.057	45.019	27.847	1.00	7.64	6
ATOM	680	C	ALA	A	84	21.758	44.332	28.688	1.00	10.46	6
ATOM	681	O	ALA	A	84	20.988	43.692	27.939	1.00	10.32	8
ATOM	682	N	ILE	A	85	21.828	44.045	29.995	1.00	10.47	7
ATOM	683	CA	ILE	A	85	21.036	42.985	30.642	1.00	10.46	6
ATOM	684	CB	ILE	A	85	21.501	42.710	32.116	1.00	9.71	6
ATOM	685	CG2	ILE	A	85	20.474	41.875	32.906	1.00	6.40	6
ATOM	686	CG1	ILE	A	85	22.921	42.132	32.080	1.00	9.01	6
ATOM	687	CD1	ILE	A	85	23.684	42.092	33.399	1.00	10.12	6
ATOM	688	C	ILE	A	85	19.543	43.282	30.566	1.00	10.65	6
ATOM	689	O	ILE	A	85	18.768	42.340	30.313	1.00	10.41	8
ATOM	690	N	GLY	A	86	19.100	44.530	30.757	1.00	11.09	7
ATOM	691	CA	GLY	A	86	17.669	44.837	30.621	1.00	11.74	6
ATOM	692	C	GLY	A	86	17.181	44.628	29.181	1.00	12.11	6
ATOM	693	O	GLY	A	86	16.109	44.068	28.922	1.00	12.28	8
ATOM	694	N	SER	A	87	17.881	45.049	28.130	1.00	12.31	7
ATOM	695	CA	SER	A	87	17.451	44.776	26.770	1.00	12.79	6
ATOM	696	CB	SER	A	87	18.466	45.329	25.735	1.00	13.98	6
ATOM	697	OG	SER	A	87	18.420	46.745	26.044	1.00	18.72	8
ATOM	698	C	SER	A	87	17.310	43.266	26.465	1.00	12.80	6
ATOM	699	O	SER	A	87	16.395	42.812	25.776	1.00	12.92	8
ATOM	700	N	LEU	A	88	18.262	42.459	26.958	1.00	12.48	7
ATOM	701	CA	LEU	A	88	18.199	41.020	26.764	1.00	12.30	6
ATOM	702	CB	LEU	A	88	19.475	40.339	27.265	1.00	11.21	6
ATOM	703	CG	LEU	A	88	20.738	40.582	26.420	1.00	10.80	6
ATOM	704	CD1	LEU	A	88	21.896	40.048	27.197	1.00	8.96	6
ATOM	705	CD2	LEU	A	88	20.566	39.947	25.036	1.00	11.89	6
ATOM	706	C	LEU	A	88	16.995	40.443	27.507	1.00	12.23	6
ATOM	707	O	LEU	A	88	16.258	39.575	26.993	1.00	12.29	8
ATOM	708	N	HIS	A	89	16.784	40.866	28.752	1.00	12.11	7
ATOM	709	CA	HIS	A	89	15.679	40.323	29.507	1.00	12.49	6
ATOM	710	CB	HIS	A	89	15.713	40.745	30.987	1.00	11.47	6
ATOM	711	CG	HIS	A	89	16.594	39.915	31.863	1.00	11.05	6
ATOM	712	CD2	HIS	A	89	17.072	38.635	31.719	1.00	11.34	6
ATOM	713	ND1	HIS	A	89	17.117	40.353	33.037	1.00	10.31	7
ATOM	714	CE1	HIS	A	89	17.865	39.425	33.593	1.00	10.84	6
ATOM	715	NE2	HIS	A	89	17.837	38.343	32.823	1.00	11.68	7
ATOM	716	C	HIS	A	89	14.378	40.741	28.838	1.00	13.05	6
ATOM	717	O	HIS	A	89	13.480	39.910	28.764	1.00	12.72	8
ATOM	718	N	SER	A	90	14.275	41.957	28.285	1.00	13.89	7
ATOM	719	CA	SER	A	90	12.957	42.281	27.665	1.00	15.19	6
ATOM	720	CB	SER	A	90	12.784	43.796	27.578	1.00	14.96	6
ATOM	721	OG	SER	A	90	13.761	44.225	26.638	1.00	19.72	8
ATOM	722	C	SER	A	90	12.722	41.472	26.411	1.00	15.94	6
ATOM	723	O	SER	A	90	11.612	41.428	25.924	1.00	15.88	8
ATOM	724	N	ARG	A	91	13.632	40.675	25.854	1.00	16.85	7
ATOM	725	CA	ARG	A	91	13.529	39.799	24.719	1.00	17.41	6
ATOM	726	CB	ARG	A	91	14.651	39.930	23.689	1.00	20.09	6
ATOM	727	CG	ARG	A	91	14.977	41.395	23.474	1.00	23.93	6
ATOM	728	CD	ARG	A	91	14.271	41.859	22.236	1.00	27.09	6
ATOM	729	NE	ARG	A	91	14.479	43.230	22.020	1.00	31.65	7
ATOM	730	CZ	ARG	A	91	15.007	44.382	22.298	1.00	33.62	6
ATOM	731	NH1	ARG	A	91	15.835	44.587	23.321	1.00	33.94	7
ATOM	732	NH2	ARG	A	91	14.682	45.428	21.512	1.00	34.30	7
ATOM	733	C	ARG	A	91	13.594	38.341	25.184	1.00	17.75	6
ATOM	734	O	ARG	A	91	13.827	37.473	24.354	1.00	17.92	8
ATOM	735	N	ASN	A	92	13.435	38.126	26.487	1.00	17.94	7
ATOM	736	CA	ASN	A	92	13.471	36.780	27.044	1.00	17.98	6
ATOM	737	CB	ASN	A	92	12.229	35.993	26.546	1.00	24.48	6
ATOM	738	CG	ASN	A	92	11.010	36.657	27.191	1.00	29.10	6
ATOM	739	OD1	ASN	A	92	10.782	36.615	28.414	1.00	31.71	8
ATOM	740	ND2	ASN	A	92	10.235	37.344	26.343	1.00	30.92	7
ATOM	741	C	ASN	A	92	14.740	35.989	26.780	1.00	17.40	6
ATOM	742	O	ASN	A	92	14.762	34.799	26.423	1.00	17.64	8

Appendix 1

ATOM	743	N	VAL	A	93	15.886	36.642	26.989	1.00	16.55	7
ATOM	744	CA	VAL	A	93	17.213	36.038	26.833	1.00	15.28	6
ATOM	745	CB	VAL	A	93	18.120	36.688	25.785	1.00	12.97	6
ATOM	746	CG1	VAL	A	93	19.467	36.021	25.589	1.00	11.55	6
ATOM	747	CG2	VAL	A	93	17.378	36.751	24.453	1.00	12.58	6
ATOM	748	C	VAL	A	93	17.771	36.161	28.256	1.00	14.60	6
ATOM	749	O	VAL	A	93	17.736	37.228	28.829	1.00	14.36	8
ATOM	750	N	GLN	A	94	18.211	35.007	28.742	1.00	13.97	7
ATOM	751	CA	GLN	A	94	18.792	34.812	30.045	1.00	13.10	6
ATOM	752	CB	GLN	A	94	18.642	33.375	30.542	1.00	13.62	6
ATOM	753	CG	GLN	A	94	17.165	33.203	30.919	1.00	16.17	6
ATOM	754	CD	GLN	A	94	17.047	31.828	31.552	1.00	19.51	6
ATOM	755	OE1	GLN	A	94	17.710	30.855	31.198	1.00	21.76	8
ATOM	756	NE2	GLN	A	94	16.206	31.683	32.559	1.00	21.21	7
ATOM	757	C	GLN	A	94	20.275	35.223	30.003	1.00	12.28	6
ATOM	758	O	GLN	A	94	20.882	35.311	28.935	1.00	12.02	8
ATOM	759	N	VAL	A	95	20.772	35.576	31.218	1.00	11.32	7
ATOM	760	CA	VAL	A	95	22.144	36.030	31.272	1.00	10.46	6
ATOM	761	CB	VAL	A	95	22.215	37.553	31.568	1.00	11.92	6
ATOM	762	CG1	VAL	A	95	23.646	38.014	31.735	1.00	12.03	6
ATOM	763	CG2	VAL	A	95	21.591	38.367	30.411	1.00	12.21	6
ATOM	764	C	VAL	A	95	22.942	35.249	32.302	1.00	9.65	6
ATOM	765	O	VAL	A	95	22.559	35.259	33.483	1.00	9.73	8
ATOM	766	N	TYR	A	96	24.034	34.613	31.857	1.00	8.90	7
ATOM	767	CA	TYR	A	96	24.920	33.882	32.786	1.00	8.34	6
ATOM	768	CB	TYR	A	96	25.217	32.512	32.267	1.00	8.31	6
ATOM	769	CG	TYR	A	96	24.055	31.583	31.987	1.00	8.37	6
ATOM	770	CD1	TYR	A	96	24.298	30.500	31.130	1.00	8.46	6
ATOM	771	CE1	TYR	A	96	23.255	29.643	30.831	1.00	8.30	6
ATOM	772	CD2	TYR	A	96	22.797	31.752	32.491	1.00	8.19	6
ATOM	773	CE2	TYR	A	96	21.742	30.928	32.186	1.00	8.05	6
ATOM	774	CZ	TYR	A	96	22.011	29.854	31.363	1.00	7.94	6
ATOM	775	OH	TYR	A	96	21.055	28.940	31.084	1.00	7.64	8
ATOM	776	C	TYR	A	96	26.218	34.655	33.000	1.00	8.00	6
ATOM	777	O	TYR	A	96	26.855	35.017	32.005	1.00	7.99	8
ATOM	778	N	GLY	A	97	26.624	34.919	34.243	1.00	7.85	7
ATOM	779	CA	GLY	A	97	27.818	35.671	34.578	1.00	7.64	6
ATOM	780	C	GLY	A	97	29.038	34.754	34.756	1.00	7.84	6
ATOM	781	O	GLY	A	97	28.950	33.655	35.307	1.00	7.51	8
ATOM	782	N	ASP	A	98	30.194	35.231	34.285	1.00	7.87	7
ATOM	783	CA	ASP	A	98	31.455	34.489	34.482	1.00	8.04	6
ATOM	784	CB	ASP	A	98	32.546	34.944	33.523	1.00	7.77	6
ATOM	785	CG	ASP	A	98	33.452	33.828	33.077	1.00	7.80	6
ATOM	786	OD1	ASP	A	98	33.916	33.045	33.920	1.00	8.28	8
ATOM	787	OD2	ASP	A	98	33.791	33.741	31.896	1.00	8.14	8
ATOM	788	C	ASP	A	98	31.868	34.668	35.953	1.00	7.80	6
ATOM	789	O	ASP	A	98	31.644	35.739	36.518	1.00	7.83	8
ATOM	790	N	VAL	A	99	32.333	33.601	36.602	1.00	7.67	7
ATOM	791	CA	VAL	A	99	32.708	33.576	38.035	1.00	7.25	6
ATOM	792	CB	VAL	A	99	31.742	32.652	38.791	1.00	8.70	6
ATOM	793	CG1	VAL	A	99	32.193	32.306	40.195	1.00	9.79	6
ATOM	794	CG2	VAL	A	99	30.366	33.362	38.885	1.00	9.90	6
ATOM	795	C	VAL	A	99	34.155	33.123	38.148	1.00	6.81	6
ATOM	796	O	VAL	A	99	34.461	31.987	37.850	1.00	6.46	8
ATOM	797	N	VAL	A	100	35.082	34.017	38.489	1.00	6.60	7
ATOM	798	CA	VAL	A	100	36.487	33.766	38.594	1.00	6.45	6
ATOM	799	CB	VAL	A	100	37.273	34.786	37.735	1.00	6.89	6
ATOM	800	CG1	VAL	A	100	38.728	34.308	37.697	1.00	6.74	6
ATOM	801	CG2	VAL	A	100	36.761	34.893	36.314	1.00	6.94	6
ATOM	802	C	VAL	A	100	36.930	33.803	40.041	1.00	6.61	6
ATOM	803	O	VAL	A	100	37.306	34.866	40.566	1.00	6.72	8
ATOM	804	N	LEU	A	101	36.882	32.651	40.724	1.00	6.41	7
ATOM	805	CA	LEU	A	101	37.189	32.537	42.133	1.00	6.10	6
ATOM	806	CB	LEU	A	101	36.017	31.716	42.731	1.00	7.20	6
ATOM	807	CG	LEU	A	101	34.663	32.479	42.645	1.00	8.90	6
ATOM	808	CD1	LEU	A	101	33.657	31.509	43.300	1.00	9.60	6
ATOM	809	CD2	LEU	A	101	34.726	33.873	43.244	1.00	7.63	6
ATOM	810	C	LEU	A	101	38.456	31.843	42.579	1.00	5.96	6
ATOM	811	O	LEU	A	101	38.672	31.740	43.782	1.00	6.02	8
ATOM	812	N	ASN	A	102	39.260	31.326	41.676	1.00	5.73	7
ATOM	813	CA	ASN	A	102	40.471	30.629	42.025	1.00	5.58	6
ATOM	814	CB	ASN	A	102	40.963	29.889	40.727	1.00	5.00	6
ATOM	815	CG	ASN	A	102	42.327	29.247	40.912	1.00	5.00	6
ATOM	816	OD1	ASN	A	102	42.309	28.218	41.608	1.00	5.00	8
ATOM	817	ND2	ASN	A	102	43.493	29.633	40.442	1.00	5.00	7
ATOM	818	C	ASN	A	102	41.580	31.490	42.620	1.00	5.69	6
ATOM	819	O	ASN	A	102	42.261	31.045	43.593	1.00	6.11	8
ATOM	820	N	HIS	A	103	41.853	32.670	42.103	1.00	5.60	7
ATOM	821	CA	HIS	A	103	42.935	33.520	42.506	1.00	5.59	6
ATOM	822	CB	HIS	A	103	44.089	33.287	41.487	1.00	6.54	6
ATOM	823	CG	HIS	A	103	43.645	33.442	40.043	1.00	7.70	6
ATOM	824	CD2	HIS	A	103	43.560	34.512	39.230	1.00	6.52	6
ATOM	825	ND1	HIS	A	103	43.187	32.341	39.282	1.00	9.01	7
ATOM	826	CE1	HIS	A	103	42.794	32.769	38.082	1.00	8.40	6
ATOM	827	NE2	HIS	A	103	42.993	34.113	38.070	1.00	8.31	7
ATOM	828	C	HIS	A	103	42.555	34.977	42.419	1.00	5.57	6
ATOM	829	O	HIS	A	103	41.470	35.229	41.899	1.00	5.20	8
ATOM	830	N	LYS	A	104	43.438	35.861	42.914	1.00	5.83	7
ATOM	831	CA	LYS	A	104	43.226	37.313	42.871	1.00	6.01	6
ATOM	832	CB	LYS	A	104	42.938	37.971	44.213	1.00	8.00	6
ATOM	833	CG	LYS	A	104	41.748	37.393	44.978	1.00	8.52	6
ATOM	834	CD	LYS	A	104	41.373	38.324	46.133	1.00	9.80	6
ATOM	835	CE	LYS	A	104	40.973	39.748	45.746	1.00	8.97	6
ATOM	836	NZ	LYS	A	104	39.514	39.723	45.383	1.00	8.50	7
ATOM	837	C	LYS	A	104	44.489	37.894	42.278	1.00	6.11	6
ATOM	838	O	LYS	A	104	45.526	37.321	42.649	1.00	6.50	8
ATOM	839	N	ALA	A	105	44.501	38.896	41.451	1.00	5.96	7
ATOM	840	CA	ALA	A	105	45.699	39.429	40.846	1.00	6.18	6
ATOM	841	CB	ALA	A	105	45.660	39.063	39.341	1.00	5.88	6
ATOM	842	C	ALA	A	105	45.785	40.943	41.031	1.00	6.37	6
ATOM	843	O	ALA	A	105	44.741	41.578	41.199	1.00	6.24	8
ATOM	844	N	GLY	A	106	46.958	41.584	41.044	1.00	6.40	7
ATOM	845	CA	GLY	A	106	47.040	43.001	41.190	1.00	6.60	6
ATOM	846	C	GLY	A	106	47.006	43.611	42.573	1.00	7.01	6
ATOM	847	O	GLY	A	106	46.524	44.736	42.659	1.00	6.76	8
ATOM	848	N	ALA	A	107	47.489	42.945	43.637	1.00	7.49	7

ATOM	849	CA	ALA	A	107	47.462	43.434	44.979	1.00	7.87	6
ATOM	850	CB	ALA	A	107	48.271	42.572	45.920	1.00	5.59	6
ATOM	851	C	ALA	A	107	48.055	44.842	44.970	1.00	8.71	6
ATOM	852	O	ALA	A	107	48.875	45.204	44.120	1.00	8.95	8
ATOM	853	N	ASP	A	108	47.647	45.649	45.934	1.00	9.17	7
ATOM	854	CA	ASP	A	108	48.106	47.011	46.130	1.00	9.77	6
ATOM	855	CB	ASP	A	108	47.118	47.666	47.155	1.00	10.59	6
ATOM	856	CG	ASP	A	108	45.718	47.703	46.582	1.00	10.42	6
ATOM	857	OD1	ASP	A	108	44.685	47.094	46.851	1.00	10.41	8
ATOM	858	OD2	ASP	A	108	45.580	48.455	45.604	1.00	12.47	8
ATOM	859	C	ASP	A	108	49.530	47.044	46.683	1.00	10.18	6
ATOM	860	O	ASP	A	108	50.281	48.011	46.478	1.00	10.34	8
ATOM	861	N	ALA	A	109	49.958	46.023	47.436	1.00	10.17	7
ATOM	862	CA	ALA	A	109	51.273	45.970	48.023	1.00	10.21	6
ATOM	863	CB	ALA	A	109	51.271	46.787	49.322	1.00	10.14	6
ATOM	864	C	ALA	A	109	51.669	44.553	48.398	1.00	10.56	6
ATOM	865	O	ALA	A	109	50.836	43.629	48.473	1.00	10.49	8
ATOM	866	N	THR	A	110	52.966	44.438	48.710	1.00	10.81	7
ATOM	867	CA	THR	A	110	53.504	43.168	49.132	1.00	11.01	6
ATOM	868	CB	THR	A	110	54.958	42.954	48.705	1.00	11.26	6
ATOM	869	OG1	THR	A	110	55.741	43.988	49.294	1.00	11.79	8
ATOM	870	CG2	THR	A	110	55.196	43.055	47.209	1.00	11.23	6
ATOM	871	C	THR	A	110	53.445	43.091	50.643	1.00	11.37	6
ATOM	872	O	THR	A	110	53.349	44.102	51.351	1.00	11.33	8
ATOM	873	N	GLU	A	111	53.477	41.851	51.165	1.00	11.70	7
ATOM	874	CA	GLU	A	111	53.527	41.504	52.566	1.00	11.89	6
ATOM	875	CB	GLU	A	111	52.223	40.870	53.035	1.00	10.98	6
ATOM	876	CG	GLU	A	111	51.153	41.995	53.103	1.00	13.17	6
ATOM	877	CD	GLU	A	111	49.812	41.428	53.483	1.00	14.55	6
ATOM	878	OE1	GLU	A	111	49.365	40.456	52.823	1.00	14.72	8
ATOM	879	OE2	GLU	A	111	49.218	41.958	54.436	1.00	15.89	8
ATOM	880	C	GLU	A	111	54.697	40.516	52.799	1.00	12.41	6
ATOM	881	O	GLU	A	111	55.011	39.715	51.878	1.00	12.22	8
ATOM	882	N	ASP	A	112	55.284	40.485	53.981	1.00	12.71	7
ATOM	883	CA	ASP	A	112	56.344	39.543	54.283	1.00	13.23	6
ATOM	884	CB	ASP	A	112	57.290	39.993	55.380	1.00	18.18	6
ATOM	885	CG	ASP	A	112	58.008	41.297	55.120	1.00	21.75	6
ATOM	886	OD1	ASP	A	112	58.435	41.747	54.039	1.00	23.40	8
ATOM	887	OD2	ASP	A	112	58.189	42.024	56.128	1.00	24.60	8
ATOM	888	C	ASP	A	112	55.666	38.250	54.730	1.00	13.29	6
ATOM	889	O	ASP	A	112	54.802	38.272	55.608	1.00	13.60	8
ATOM	890	N	VAL	A	113	56.015	37.098	54.155	1.00	13.04	7
ATOM	891	CA	VAL	A	113	55.381	35.819	54.410	1.00	12.72	6
ATOM	892	CB	VAL	A	113	54.466	35.495	53.205	1.00	13.86	6
ATOM	893	CG1	VAL	A	113	53.650	34.192	53.418	1.00	14.55	6
ATOM	894	CG2	VAL	A	113	53.423	36.541	52.806	1.00	13.68	6
ATOM	895	C	VAL	A	113	56.407	34.721	54.511	1.00	12.52	6
ATOM	896	O	VAL	A	113	57.412	34.748	53.765	1.00	12.66	8
ATOM	897	N	THR	A	114	56.238	33.728	55.355	1.00	12.21	7
ATOM	898	CA	THR	A	114	57.167	32.595	55.443	1.00	11.87	6
ATOM	899	CB	THR	A	114	57.212	31.941	56.800	1.00	12.24	6
ATOM	900	OG1	THR	A	114	57.602	32.955	57.741	1.00	14.04	8
ATOM	901	CG2	THR	A	114	58.195	30.781	56.909	1.00	10.63	6
ATOM	902	C	THR	A	114	56.563	31.547	54.495	1.00	11.69	6
ATOM	903	O	THR	A	114	55.355	31.265	54.457	1.00	11.32	8
ATOM	904	N	ALA	A	115	57.429	31.042	53.643	1.00	11.64	7
ATOM	905	CA	ALA	A	115	57.024	30.048	52.638	1.00	11.55	6
ATOM	906	CB	ALA	A	115	56.825	30.894	51.357	1.00	10.80	6
ATOM	907	C	ALA	A	115	58.039	28.947	52.343	1.00	11.45	6
ATOM	908	O	ALA	A	115	59.215	29.073	52.688	1.00	11.41	8
ATOM	909	N	VAL	A	116	57.641	27.868	51.657	1.00	11.33	7
ATOM	910	CA	VAL	A	116	58.513	26.814	51.184	1.00	11.10	6
ATOM	911	CB	VAL	A	116	58.338	25.436	51.815	1.00	12.01	6
ATOM	912	CG1	VAL	A	116	58.978	25.449	53.208	1.00	12.23	6
ATOM	913	CG2	VAL	A	116	56.882	24.978	51.873	1.00	11.15	6
ATOM	914	C	VAL	A	116	58.250	26.642	49.656	1.00	10.95	6
ATOM	915	O	VAL	A	116	57.100	26.960	49.240	1.00	11.03	8
ATOM	916	N	GLU	A	117	59.187	26.205	48.856	1.00	10.29	7
ATOM	917	CA	GLU	A	117	58.932	25.898	47.465	1.00	10.06	6
ATOM	918	CB	GLU	A	117	60.201	25.861	46.625	1.00	11.90	6
ATOM	919	CG	GLU	A	117	60.905	27.201	46.773	1.00	14.30	6
ATOM	920	CD	GLU	A	117	62.245	27.143	46.070	1.00	16.13	6
ATOM	921	OE1	GLU	A	117	62.515	26.342	45.175	1.00	16.80	8
ATOM	922	OE2	GLU	A	117	63.067	28.004	46.366	1.00	17.32	8
ATOM	923	C	GLU	A	117	58.354	24.480	47.369	1.00	9.67	6
ATOM	924	O	GLU	A	117	58.596	23.656	48.258	1.00	9.47	8
ATOM	925	N	VAL	A	118	57.623	24.157	46.316	1.00	9.40	7
ATOM	926	CA	VAL	A	118	56.987	22.802	46.152	1.00	9.25	6
ATOM	927	CB	VAL	A	118	55.556	23.243	46.543	1.00	10.55	6
ATOM	928	CG1	VAL	A	118	54.529	23.164	45.421	1.00	9.52	6
ATOM	929	CG2	VAL	A	118	55.061	22.664	47.855	1.00	10.49	6
ATOM	930	C	VAL	A	118	57.360	22.305	44.765	1.00	9.31	6
ATOM	931	O	VAL	A	118	57.660	23.097	43.823	1.00	9.23	8
ATOM	932	N	ASN	A	119	57.381	20.998	44.492	1.00	8.84	7
ATOM	933	CA	ASN	A	119	57.701	20.403	43.206	1.00	8.20	6
ATOM	934	CB	ASN	A	119	57.911	18.914	43.534	1.00	7.82	6
ATOM	935	CG	ASN	A	119	58.248	18.097	42.289	1.00	8.10	6
ATOM	936	OD1	ASN	A	119	58.084	18.636	41.177	1.00	7.16	8
ATOM	937	ND2	ASN	A	119	58.706	16.848	42.386	1.00	6.98	7
ATOM	938	C	ASN	A	119	56.553	20.692	42.242	1.00	7.98	6
ATOM	939	O	ASN	A	119	55.382	20.414	42.482	1.00	7.64	8
ATOM	940	N	PRO	A	120	56.833	21.326	41.094	1.00	8.04	7
ATOM	941	CD	PRO	A	120	58.207	21.735	40.728	1.00	8.00	6
ATOM	942	CA	PRO	A	120	55.849	21.704	40.088	1.00	8.27	6
ATOM	943	CB	PRO	A	120	56.609	22.404	38.938	1.00	8.21	6
ATOM	944	CG	PRO	A	120	57.980	22.618	39.530	1.00	8.16	6
ATOM	945	C	PRO	A	120	55.032	20.526	39.601	1.00	8.65	6
ATOM	946	O	PRO	A	120	53.858	20.633	39.275	1.00	8.69	8
ATOM	947	N	ALA	A	121	55.648	19.337	39.540	1.00	9.00	7
ATOM	948	CA	ALA	A	121	54.977	18.104	39.122	1.00	9.39	6
ATOM	949	CB	ALA	A	121	55.976	17.215	38.324	1.00	9.49	6
ATOM	950	C	ALA	A	121	54.374	17.315	40.267	1.00	9.46	6
ATOM	951	O	ALA	A	121	53.644	16.327	40.066	1.00	9.60	8
ATOM	952	N	ASN	A	122	54.624	17.656	41.537	1.00	9.45	7
ATOM	953	CA	ASN	A	122	54.040	16.971	42.679	1.00	9.32	6
ATOM	954	CB	ASN	A	122	54.881	15.802	43.207	1.00	10.30	6

ATOM	955	CG	ASN	A	122	54.009	15.047	44.180	1.00	13.39	6
ATOM	956	OD1	ASN	A	122	53.085	15.591	44.786	1.00	13.50	8
ATOM	957	ND2	ASN	A	122	54.211	13.733	44.357	1.00	16.10	7
ATOM	958	C	ASN	A	122	53.936	18.050	43.742	1.00	9.22	6
ATOM	959	O	ASN	A	122	54.881	18.130	44.566	1.00	9.02	8
ATOM	960	N	ARG	A	123	52.869	18.855	43.722	1.00	9.27	7
ATOM	961	CA	ARG	A	123	52.764	19.983	44.684	1.00	9.23	6
ATOM	962	CB	ARG	A	123	51.675	20.969	44.227	1.00	7.86	6
ATOM	963	CG	ARG	A	123	52.067	21.746	42.991	1.00	6.67	6
ATOM	964	CD	ARG	A	123	51.511	21.080	41.764	1.00	6.95	6
ATOM	965	NE	ARG	A	123	51.759	21.959	40.604	1.00	9.73	7
ATOM	966	CZ	ARG	A	123	50.906	22.937	40.275	1.00	10.25	6
ATOM	967	NH1	ARG	A	123	49.828	23.054	41.044	1.00	9.79	7
ATOM	968	NH2	ARG	A	123	51.000	23.793	39.273	1.00	10.20	7
ATOM	969	C	ARG	A	123	52.593	19.557	46.158	1.00	9.23	6
ATOM	970	O	ARG	A	123	52.622	20.374	47.085	1.00	8.71	8
ATOM	971	N	ASN	A	124	52.408	18.256	46.379	1.00	9.56	7
ATOM	972	CA	ASN	A	124	52.351	17.706	47.712	1.00	10.31	6
ATOM	973	CB	ASN	A	124	51.742	16.299	47.800	1.00	11.34	6
ATOM	974	CG	ASN	A	124	50.275	16.347	47.455	1.00	14.21	6
ATOM	975	OD1	ASN	A	124	49.565	17.271	47.867	1.00	14.26	8
ATOM	976	ND2	ASN	A	124	49.887	15.391	46.590	1.00	16.51	7
ATOM	977	C	ASN	A	124	53.796	17.564	48.243	1.00	10.74	6
ATOM	978	O	ASN	A	124	53.926	17.342	49.439	1.00	10.85	8
ATOM	979	N	GLN	A	125	54.872	17.660	47.433	1.00	10.96	7
ATOM	980	CA	GLN	A	125	56.223	17.549	47.925	1.00	11.21	6
ATOM	981	CB	GLN	A	125	57.169	16.823	46.919	1.00	9.50	6
ATOM	982	CG	GLN	A	125	58.582	16.600	47.498	1.00	8.17	6
ATOM	983	CD	GLN	A	125	59.546	16.199	46.402	1.00	8.01	6
ATOM	984	OE1	GLN	A	125	59.184	16.310	45.207	1.00	6.56	8
ATOM	985	NE2	GLN	A	125	60.762	15.784	46.738	1.00	6.20	7
ATOM	986	C	GLN	A	125	56.871	18.915	48.156	1.00	11.48	6
ATOM	987	O	GLN	A	125	56.960	19.609	47.146	1.00	11.44	8
ATOM	988	N	GLU	A	126	57.345	19.217	49.360	1.00	11.79	7
ATOM	989	CA	GLU	A	126	58.053	20.468	49.610	1.00	12.46	6
ATOM	990	CB	GLU	A	126	58.042	20.856	51.115	1.00	11.31	6
ATOM	991	CG	GLU	A	126	56.589	20.799	51.582	1.00	12.45	6
ATOM	992	CD	GLU	A	126	56.371	21.288	52.993	1.00	13.36	6
ATOM	993	OE1	GLU	A	126	57.329	21.471	53.748	1.00	13.22	8
ATOM	994	OE2	GLU	A	126	55.214	21.519	53.374	1.00	14.72	8
ATOM	995	C	GLU	A	126	59.513	20.293	49.195	1.00	13.18	6
ATOM	996	O	GLU	A	126	60.198	19.292	49.513	1.00	12.98	8
ATOM	997	N	THR	A	127	60.045	21.216	48.430	1.00	14.11	7
ATOM	998	CA	THR	A	127	61.407	21.048	47.954	1.00	15.19	6
ATOM	999	CB	THR	A	127	61.487	21.193	46.420	1.00	14.68	6
ATOM	1000	OG1	THR	A	127	60.732	22.349	46.071	1.00	15.49	8
ATOM	1001	CG2	THR	A	127	60.902	19.957	45.774	1.00	13.94	6
ATOM	1002	C	THR	A	127	62.377	21.993	48.614	1.00	16.26	6
ATOM	1003	O	THR	A	127	63.552	21.851	48.283	1.00	16.67	8
ATOM	1004	N	SER	A	128	62.015	22.892	49.503	1.00	16.75	7
ATOM	1005	CA	SER	A	128	63.000	23.747	50.125	1.00	17.24	6
ATOM	1006	CB	SER	A	128	63.016	25.141	49.511	1.00	15.04	6
ATOM	1007	OG	SER	A	128	61.873	25.859	49.965	1.00	13.39	8
ATOM	1008	C	SER	A	128	62.620	23.784	51.617	1.00	18.11	6
ATOM	1009	O	SER	A	128	61.642	23.256	52.161	1.00	17.96	8
ATOM	1010	N	GLU	A	129	63.523	24.444	52.326	1.00	18.90	7
ATOM	1011	CA	GLU	A	129	63.395	24.747	53.735	1.00	19.85	6
ATOM	1012	CB	GLU	A	129	64.718	25.038	54.440	1.00	27.78	6
ATOM	1013	CG	GLU	A	129	64.794	24.360	55.817	1.00	35.30	6
ATOM	1014	CD	GLU	A	129	65.311	22.937	55.587	1.00	40.42	6
ATOM	1015	OE1	GLU	A	129	66.375	22.846	54.891	1.00	43.75	8
ATOM	1016	OE2	GLU	A	129	64.637	21.983	56.055	1.00	42.88	8
ATOM	1017	C	GLU	A	129	62.566	26.060	53.737	1.00	19.69	6
ATOM	1018	O	GLU	A	129	62.573	26.773	52.713	1.00	19.50	8
ATOM	1019	N	GLU	A	130	61.925	26.390	54.849	1.00	19.52	7
ATOM	1020	CA	GLU	A	130	61.150	27.612	54.769	1.00	19.43	6
ATOM	1021	CB	GLU	A	130	60.090	27.530	55.847	1.00	23.57	6
ATOM	1022	CG	GLU	A	130	60.633	27.773	57.215	1.00	26.39	6
ATOM	1023	CD	GLU	A	130	59.542	27.368	58.202	1.00	29.94	6
ATOM	1024	OE1	GLU	A	130	59.493	28.140	59.202	1.00	33.34	8
ATOM	1025	OE2	GLU	A	130	58.779	26.388	58.051	1.00	30.50	8
ATOM	1026	C	GLU	A	130	61.988	28.851	54.837	1.00	18.97	6
ATOM	1027	O	GLU	A	130	63.023	28.894	55.454	1.00	19.04	8
ATOM	1028	N	TYR	A	131	61.506	29.854	54.117	1.00	18.45	7
ATOM	1029	CA	TYR	A	131	62.186	31.164	54.098	1.00	17.87	6
ATOM	1030	CB	TYR	A	131	63.336	31.254	53.126	1.00	18.14	6
ATOM	1031	CG	TYR	A	131	63.123	31.022	51.656	1.00	18.56	6
ATOM	1032	CD1	TYR	A	131	63.015	32.108	50.786	1.00	18.80	6
ATOM	1033	CE1	TYR	A	131	62.837	31.915	49.415	1.00	18.78	6
ATOM	1034	CD2	TYR	A	131	63.053	29.741	51.125	1.00	18.56	6
ATOM	1035	CE2	TYR	A	131	62.856	29.566	49.772	1.00	18.73	6
ATOM	1036	CZ	TYR	A	131	62.753	30.638	48.908	1.00	18.74	6
ATOM	1037	OH	TYR	A	131	62.618	30.432	47.547	1.00	18.62	8
ATOM	1038	C	TYR	A	131	61.150	32.287	53.841	1.00	17.13	6
ATOM	1039	O	TYR	A	131	59.992	32.053	53.530	1.00	16.72	8
ATOM	1040	N	GLN	A	132	61.601	33.503	54.011	1.00	16.51	7
ATOM	1041	CA	GLN	A	132	60.855	34.718	53.865	1.00	16.10	6
ATOM	1042	CB	GLN	A	132	61.459	35.882	54.723	1.00	22.79	6
ATOM	1043	CG	GLN	A	132	60.607	35.969	55.997	1.00	29.13	6
ATOM	1044	CD	GLN	A	132	61.036	34.850	56.938	1.00	33.56	6
ATOM	1045	OE1	GLN	A	132	62.246	34.859	57.308	1.00	37.13	8
ATOM	1046	NE2	GLN	A	132	60.138	33.934	57.337	1.00	34.32	7
ATOM	1047	C	GLN	A	132	60.810	35.316	52.481	1.00	15.05	6
ATOM	1048	O	GLN	A	132	61.881	35.620	51.931	1.00	15.27	8
ATOM	1049	N	ILE	A	133	59.589	35.505	51.972	1.00	13.86	7
ATOM	1050	CA	ILE	A	133	59.481	36.102	50.631	1.00	12.62	6
ATOM	1051	CB	ILE	A	133	58.828	35.111	49.616	1.00	11.38	6
ATOM	1052	CG2	ILE	A	133	59.610	33.787	49.469	1.00	9.01	6
ATOM	1053	CG1	ILE	A	133	57.374	34.744	49.978	1.00	11.33	6
ATOM	1054	CD1	ILE	A	133	56.601	33.908	48.958	1.00	11.24	6
ATOM	1055	C	ILE	A	133	58.652	37.381	50.761	1.00	11.82	6
ATOM	1056	O	ILE	A	133	58.026	37.593	51.790	1.00	11.18	8
ATOM	1057	N	LYS	A	134	58.611	38.192	49.709	1.00	11.45	7
ATOM	1058	CA	LYS	A	134	57.737	39.379	49.674	1.00	11.11	6
ATOM	1059	CB	LYS	A	134	58.443	40.661	49.331	1.00	12.71	6
ATOM	1060	CG	LYS	A	134	59.019	41.223	50.642	1.00	15.80	6

ATOM	1061	CD	LYS	A	134	59.998	42.325	50.294	1.00	19.11	6
ATOM	1062	CE	LYS	A	134	59.652	43.476	51.253	1.00	22.58	6
ATOM	1063	NZ	LYS	A	134	59.863	42.966	52.656	1.00	24.21	7
ATOM	1064	C	LYS	A	134	56.683	39.046	48.618	1.00	10.75	6
ATOM	1065	O	LYS	A	134	57.075	38.997	47.439	1.00	10.72	8
ATOM	1066	N	ALA	A	135	55.444	38.754	48.993	1.00	10.26	7
ATOM	1067	CA	ALA	A	135	54.411	38.356	48.046	1.00	9.82	6
ATOM	1068	CB	ALA	A	135	53.713	37.071	48.552	1.00	8.45	6
ATOM	1069	C	ALA	A	135	53.360	39.428	47.848	1.00	9.62	6
ATOM	1070	O	ALA	A	135	53.052	40.158	48.834	1.00	9.91	8
ATOM	1071	N	TRP	A	136	52.718	39.492	46.672	1.00	9.28	7
ATOM	1072	CA	TRP	A	136	51.676	40.473	46.354	1.00	8.76	6
ATOM	1073	CB	TRP	A	136	51.683	40.690	44.846	1.00	9.45	6
ATOM	1074	CG	TRP	A	136	52.918	41.438	44.430	1.00	12.78	6
ATOM	1075	CD2	TRP	A	136	53.068	42.881	44.426	1.00	13.09	6
ATOM	1076	CE2	TRP	A	136	54.343	43.162	43.888	1.00	14.31	6
ATOM	1077	CE3	TRP	A	136	52.224	43.924	44.799	1.00	11.71	6
ATOM	1078	CD1	TRP	A	136	54.098	40.924	43.934	1.00	13.83	6
ATOM	1079	NE1	TRP	A	136	54.954	41.951	43.599	1.00	15.49	7
ATOM	1080	CZ2	TRP	A	136	54.846	44.456	43.772	1.00	14.17	6
ATOM	1081	CZ3	TRP	A	136	52.680	45.213	44.627	1.00	12.36	6
ATOM	1082	CH2	TRP	A	136	53.971	45.463	44.144	1.00	13.78	6
ATOM	1083	C	TRP	A	136	50.338	39.995	46.811	1.00	8.40	6
ATOM	1084	O	TRP	A	136	49.535	39.452	46.066	1.00	8.39	8
ATOM	1085	N	THR	A	137	50.028	40.192	48.086	1.00	8.12	7
ATOM	1086	CA	THR	A	137	48.844	39.707	48.761	1.00	7.75	6
ATOM	1087	CB	THR	A	137	49.275	38.704	49.884	1.00	7.93	6
ATOM	1088	OG1	THR	A	137	50.351	39.218	50.701	1.00	8.77	8
ATOM	1089	CG2	THR	A	137	49.847	37.387	49.327	1.00	8.10	6
ATOM	1090	C	THR	A	137	48.040	40.772	49.490	1.00	7.59	6
ATOM	1091	O	THR	A	137	47.063	40.370	50.112	1.00	7.09	8
ATOM	1092	N	ASP	A	138	48.425	42.026	49.486	1.00	7.55	7
ATOM	1093	CA	ASP	A	138	47.680	43.038	50.221	1.00	7.91	6
ATOM	1094	CB	ASP	A	138	48.667	44.060	50.793	1.00	10.34	6
ATOM	1095	CG	ASP	A	138	48.054	45.085	51.742	1.00	14.50	6
ATOM	1096	OD1	ASP	A	138	46.820	45.294	51.881	1.00	14.46	8
ATOM	1097	OD2	ASP	A	138	48.845	45.781	52.416	1.00	16.18	8
ATOM	1098	C	ASP	A	138	46.627	43.671	49.316	1.00	8.01	6
ATOM	1099	O	ASP	A	138	47.039	44.379	48.405	1.00	7.97	8
ATOM	1100	N	PHE	A	139	45.334	43.427	49.520	1.00	8.44	7
ATOM	1101	CA	PHE	A	139	44.298	44.016	48.652	1.00	9.00	6
ATOM	1102	CB	PHE	A	139	43.394	43.011	47.964	1.00	7.03	6
ATOM	1103	CG	PHE	A	139	44.078	42.176	46.892	1.00	8.72	6
ATOM	1104	CD1	PHE	A	139	44.948	41.138	47.287	1.00	7.30	6
ATOM	1105	CD2	PHE	A	139	43.835	42.398	45.538	1.00	7.95	6
ATOM	1106	CE1	PHE	A	139	45.600	40.359	46.350	1.00	8.84	6
ATOM	1107	CE2	PHE	A	139	44.469	41.605	44.591	1.00	8.85	6
ATOM	1108	CZ	PHE	A	139	45.335	40.593	44.979	1.00	9.11	6
ATOM	1109	C	PHE	A	139	43.461	44.987	49.487	1.00	9.73	6
ATOM	1110	O	PHE	A	139	42.707	44.536	50.343	1.00	9.71	8
ATOM	1111	N	ARG	A	140	43.599	46.294	49.178	1.00	10.52	7
ATOM	1112	CA	ARG	A	140	42.823	47.246	49.985	1.00	11.46	6
ATOM	1113	CB	ARG	A	140	43.647	48.263	50.745	1.00	17.79	6
ATOM	1114	CG	ARG	A	140	45.059	48.594	50.380	1.00	22.69	6
ATOM	1115	CD	ARG	A	140	45.796	48.583	51.753	1.00	27.78	6
ATOM	1116	NE	ARG	A	140	47.197	48.785	51.626	1.00	32.35	7
ATOM	1117	CZ	ARG	A	140	48.476	48.985	51.487	1.00	34.38	6
ATOM	1118	NH1	ARG	A	140	48.873	49.714	50.421	1.00	34.62	7
ATOM	1119	NH2	ARG	A	140	49.440	48.518	52.329	1.00	34.86	7
ATOM	1120	C	ARG	A	140	41.766	48.037	49.205	1.00	11.28	6
ATOM	1121	O	ARG	A	140	40.965	48.699	49.916	1.00	11.54	8
ATOM	1122	N	PHE	A	141	41.672	47.993	47.908	1.00	10.83	7
ATOM	1123	CA	PHE	A	141	40.554	48.658	47.231	1.00	10.94	6
ATOM	1124	CB	PHE	A	141	39.237	47.897	47.618	1.00	8.15	6
ATOM	1125	CG	PHE	A	141	39.346	46.381	47.561	1.00	6.78	6
ATOM	1126	CD1	PHE	A	141	39.041	45.616	48.673	1.00	5.88	6
ATOM	1127	CD2	PHE	A	141	39.793	45.725	46.453	1.00	5.72	6
ATOM	1128	CE1	PHE	A	141	39.150	44.225	48.627	1.00	6.27	6
ATOM	1129	CE2	PHE	A	141	39.930	44.318	46.407	1.00	5.00	6
ATOM	1130	CZ	PHE	A	141	39.607	43.584	47.478	1.00	5.00	6
ATOM	1131	C	PHE	A	141	40.372	50.134	47.543	1.00	11.05	6
ATOM	1132	O	PHE	A	141	39.377	50.553	48.103	1.00	10.80	8
ATOM	1133	N	PRO	A	142	41.402	50.934	47.254	1.00	11.32	7
ATOM	1134	CD	PRO	A	142	42.645	50.440	46.634	1.00	11.43	6
ATOM	1135	CA	PRO	A	142	41.462	52.384	47.515	1.00	11.27	6
ATOM	1136	CB	PRO	A	142	42.900	52.829	47.190	1.00	11.50	6
ATOM	1137	CG	PRO	A	142	43.300	51.728	46.191	1.00	11.68	6
ATOM	1138	C	PRO	A	142	40.424	53.179	46.766	1.00	11.03	6
ATOM	1139	O	PRO	A	142	39.933	54.100	47.431	1.00	11.24	8
ATOM	1140	N	GLY	A	143	39.984	52.964	45.545	1.00	10.61	7
ATOM	1141	CA	GLY	A	143	38.950	53.703	44.905	1.00	10.26	6
ATOM	1142	C	GLY	A	143	37.544	53.272	45.330	1.00	10.29	6
ATOM	1143	O	GLY	A	143	36.578	54.011	45.134	1.00	10.11	8
ATOM	1144	N	ARG	A	144	37.337	52.102	45.941	1.00	10.41	7
ATOM	1145	CA	ARG	A	144	36.034	51.630	46.365	1.00	10.66	6
ATOM	1146	CB	ARG	A	144	35.855	50.122	46.066	1.00	6.45	6
ATOM	1147	CG	ARG	A	144	34.545	49.572	46.609	1.00	6.10	6
ATOM	1148	CD	ARG	A	144	34.074	48.222	46.139	1.00	6.59	6
ATOM	1149	NE	ARG	A	144	35.003	47.110	46.397	1.00	7.45	7
ATOM	1150	CZ	ARG	A	144	35.062	46.377	47.500	1.00	7.53	6
ATOM	1151	NH1	ARG	A	144	35.983	45.402	47.626	1.00	8.54	7
ATOM	1152	NH2	ARG	A	144	34.219	46.599	48.511	1.00	6.60	7
ATOM	1153	C	ARG	A	144	35.736	51.908	47.869	1.00	11.31	6
ATOM	1154	O	ARG	A	144	34.643	52.176	48.348	1.00	11.05	8
ATOM	1155	N	GLY	A	145	36.813	51.804	48.658	1.00	11.78	7
ATOM	1156	CA	GLY	A	145	36.758	51.954	50.104	1.00	12.35	6
ATOM	1157	C	GLY	A	145	35.922	50.757	50.584	1.00	12.97	6
ATOM	1158	O	GLY	A	145	36.169	49.601	50.164	1.00	13.33	8
ATOM	1159	N	ASN	A	146	34.906	51.057	51.416	1.00	12.95	7
ATOM	1160	CA	ASN	A	146	34.070	49.991	51.970	1.00	12.83	6
ATOM	1161	CB	ASN	A	146	33.889	50.195	53.493	1.00	15.58	6
ATOM	1162	CG	ASN	A	146	35.151	49.936	54.288	1.00	19.40	6
ATOM	1163	OD1	ASN	A	146	36.065	49.159	53.989	1.00	20.79	8
ATOM	1164	ND2	ASN	A	146	35.264	50.678	55.410	1.00	20.44	7
ATOM	1165	C	ASN	A	146	32.689	49.855	51.336	1.00	12.13	6
ATOM	1166	O	ASN	A	146	31.905	49.168	52.002	1.00	12.08	8

ATOM	1167	N	THR	A	147	32.491	50.456	50.175	1.00	11.60	7
ATOM	1168	CA	THR	A	147	31.200	50.351	49.487	1.00	11.26	6
ATOM	1169	CB	THR	A	147	31.164	51.128	48.161	1.00	11.45	6
ATOM	1170	OG1	THR	A	147	31.709	52.445	48.360	1.00	12.12	8
ATOM	1171	CG2	THR	A	147	29.782	51.325	47.548	1.00	9.27	6
ATOM	1172	C	THR	A	147	30.895	48.884	49.247	1.00	11.00	6
ATOM	1173	O	THR	A	147	31.757	48.136	48.721	1.00	11.07	8
ATOM	1174	N	TYR	A	148	29.718	48.430	49.662	1.00	10.51	7
ATOM	1175	CA	TYR	A	148	29.245	47.066	49.538	1.00	10.34	6
ATOM	1176	CB	TYR	A	148	29.308	46.455	48.113	1.00	10.35	6
ATOM	1177	CG	TYR	A	148	28.798	47.326	46.967	1.00	9.97	6
ATOM	1178	CD1	TYR	A	148	29.649	47.666	45.916	1.00	9.49	6
ATOM	1179	CE1	TYR	A	148	29.177	48.430	44.845	1.00	9.11	6
ATOM	1180	CD2	TYR	A	148	27.474	47.843	46.971	1.00	9.73	6
ATOM	1181	CE2	TYR	A	148	27.047	48.636	45.925	1.00	9.48	6
ATOM	1182	CZ	TYR	A	148	27.896	48.914	44.844	1.00	8.99	6
ATOM	1183	OH	TYR	A	148	27.441	49.705	43.833	1.00	8.37	8
ATOM	1184	C	TYR	A	148	29.940	46.030	50.426	1.00	10.22	6
ATOM	1185	O	TYR	A	148	29.299	45.054	50.827	1.00	10.08	8
ATOM	1186	N	SER	A	149	31.224	46.159	50.757	1.00	10.07	7
ATOM	1187	CA	SER	A	149	31.879	45.141	51.584	1.00	9.72	6
ATOM	1188	CB	SER	A	149	32.256	43.886	50.787	1.00	9.55	6
ATOM	1189	OG	SER	A	149	33.396	43.185	51.181	1.00	8.96	8
ATOM	1190	C	SER	A	149	33.141	45.735	52.164	1.00	9.63	6
ATOM	1191	O	SER	A	149	33.897	46.334	51.423	1.00	9.31	8
ATOM	1192	N	ASP	A	150	33.270	45.588	53.502	1.00	9.75	7
ATOM	1193	CA	ASP	A	150	34.497	46.155	54.053	1.00	9.98	6
ATOM	1194	CB	ASP	A	150	34.153	46.816	55.365	1.00	13.89	6
ATOM	1195	CG	ASP	A	150	33.646	45.849	56.403	1.00	17.64	6
ATOM	1196	OD1	ASP	A	150	33.340	44.644	56.213	1.00	18.84	8
ATOM	1197	OD2	ASP	A	150	33.560	46.260	57.579	1.00	20.98	8
ATOM	1198	C	ASP	A	150	35.545	45.049	54.125	1.00	9.95	6
ATOM	1199	O	ASP	A	150	36.570	45.334	54.761	1.00	10.38	8
ATOM	1200	N	PHE	A	151	35.472	43.865	53.541	1.00	9.49	7
ATOM	1201	CA	PHE	A	151	36.518	42.860	53.667	1.00	8.88	6
ATOM	1202	CB	PHE	A	151	35.932	41.523	53.167	1.00	10.40	6
ATOM	1203	CG	PHE	A	151	36.761	40.297	53.405	1.00	12.18	6
ATOM	1204	CD1	PHE	A	151	36.689	39.627	54.620	1.00	14.04	6
ATOM	1205	CD2	PHE	A	151	37.623	39.804	52.455	1.00	12.75	6
ATOM	1206	CE1	PHE	A	151	37.481	38.471	54.849	1.00	15.14	6
ATOM	1207	CE2	PHE	A	151	38.380	38.647	52.644	1.00	12.08	6
ATOM	1208	CZ	PHE	A	151	38.308	37.976	53.849	1.00	13.39	6
ATOM	1209	C	PHE	A	151	37.748	43.217	52.864	1.00	8.54	6
ATOM	1210	O	PHE	A	151	37.762	43.556	51.675	1.00	8.21	8
ATOM	1211	N	LYS	A	152	38.899	43.119	53.477	1.00	8.50	7
ATOM	1212	CA	LYS	A	152	40.228	43.377	52.979	1.00	8.62	6
ATOM	1213	CB	LYS	A	152	40.989	44.385	53.849	1.00	10.86	6
ATOM	1214	CG	LYS	A	152	40.384	45.787	54.073	1.00	11.07	6
ATOM	1215	CD	LYS	A	152	39.941	46.481	52.798	1.00	11.11	6
ATOM	1216	CE	LYS	A	152	39.350	47.830	53.236	1.00	12.45	6
ATOM	1217	NZ	LYS	A	152	38.434	48.440	52.290	1.00	15.39	7
ATOM	1218	C	LYS	A	152	41.038	42.082	52.958	1.00	8.53	6
ATOM	1219	O	LYS	A	152	40.938	41.290	53.892	1.00	8.53	8
ATOM	1220	N	TRP	A	153	41.841	41.875	51.926	1.00	8.13	7
ATOM	1221	CA	TRP	A	153	42.585	40.644	51.805	1.00	7.85	6
ATOM	1222	CB	TRP	A	153	42.567	40.241	50.293	1.00	6.88	6
ATOM	1223	CG	TRP	A	153	41.174	39.851	49.872	1.00	6.70	6
ATOM	1224	CD2	TRP	A	153	40.681	38.522	49.679	1.00	6.38	6
ATOM	1225	CE2	TRP	A	153	39.330	38.637	49.270	1.00	7.85	6
ATOM	1226	CE3	TRP	A	153	41.225	37.236	49.779	1.00	6.59	6
ATOM	1227	CD1	TRP	A	153	40.139	40.695	49.600	1.00	6.77	6
ATOM	1228	NE1	TRP	A	153	39.018	39.986	49.233	1.00	6.86	7
ATOM	1229	CZ2	TRP	A	153	38.542	37.504	48.986	1.00	7.93	6
ATOM	1230	CZ3	TRP	A	153	40.477	36.113	49.452	1.00	7.12	6
ATOM	1231	CH2	TRP	A	153	39.128	36.250	49.081	1.00	8.55	6
ATOM	1232	C	TRP	A	153	44.014	40.738	52.256	1.00	7.70	6
ATOM	1233	O	TRP	A	153	44.633	41.770	52.009	1.00	7.54	8
ATOM	1234	N	HIS	A	154	44.568	39.706	52.892	1.00	7.67	7
ATOM	1235	CA	HIS	A	154	45.937	39.586	53.334	1.00	7.24	6
ATOM	1236	CB	HIS	A	154	46.112	39.730	54.859	1.00	7.92	6
ATOM	1237	CG	HIS	A	154	45.804	41.145	55.233	1.00	8.88	6
ATOM	1238	CD2	HIS	A	154	44.674	41.660	55.765	1.00	9.84	6
ATOM	1239	ND1	HIS	A	154	46.672	42.197	55.006	1.00	10.11	7
ATOM	1240	CE1	HIS	A	154	46.113	43.304	55.428	1.00	10.55	6
ATOM	1241	NE2	HIS	A	154	44.890	43.016	55.840	1.00	10.76	7
ATOM	1242	C	HIS	A	154	46.508	38.207	52.960	1.00	6.90	6
ATOM	1243	O	HIS	A	154	45.778	37.294	52.603	1.00	6.75	8
ATOM	1244	N	TRP	A	155	47.839	38.056	53.102	1.00	6.82	7
ATOM	1245	CA	TRP	A	155	48.508	36.802	52.800	1.00	6.92	6
ATOM	1246	CB	TRP	A	155	49.994	36.800	53.254	1.00	6.54	6
ATOM	1247	CG	TRP	A	155	50.190	36.808	54.726	1.00	6.55	6
ATOM	1248	CD2	TRP	A	155	50.282	35.636	55.575	1.00	7.16	6
ATOM	1249	CE2	TRP	A	155	50.473	36.099	56.900	1.00	8.10	6
ATOM	1250	CE3	TRP	A	155	50.261	34.254	55.319	1.00	7.58	6
ATOM	1251	CD1	TRP	A	155	50.311	37.912	55.567	1.00	7.09	6
ATOM	1252	NE1	TRP	A	155	50.496	37.495	56.870	1.00	7.83	7
ATOM	1253	CZ2	TRP	A	155	50.582	35.208	57.972	1.00	9.47	6
ATOM	1254	CZ3	TRP	A	155	50.372	33.377	56.355	1.00	8.70	6
ATOM	1255	CH2	TRP	A	155	50.556	33.847	57.685	1.00	9.74	6
ATOM	1256	C	TRP	A	155	47.807	35.600	53.420	1.00	6.90	6
ATOM	1257	O	TRP	A	155	47.749	34.576	52.755	1.00	6.82	8
ATOM	1258	N	TYR	A	156	47.293	35.659	54.655	1.00	6.91	7
ATOM	1259	CA	TYR	A	156	46.692	34.492	55.283	1.00	6.91	6
ATOM	1260	CB	TYR	A	156	46.619	34.685	56.813	1.00	7.50	6
ATOM	1261	CG	TYR	A	156	46.056	36.003	57.270	1.00	8.16	6
ATOM	1262	CD1	TYR	A	156	44.665	36.114	57.420	1.00	8.64	6
ATOM	1263	CE1	TYR	A	156	44.049	37.302	57.839	1.00	8.68	6
ATOM	1264	CD2	TYR	A	156	46.829	37.094	57.597	1.00	8.54	6
ATOM	1265	CE2	TYR	A	156	46.254	38.298	58.052	1.00	8.83	6
ATOM	1266	CZ	TYR	A	156	44.870	38.365	58.159	1.00	8.97	6
ATOM	1267	OH	TYR	A	156	44.271	39.510	58.597	1.00	9.48	8
ATOM	1268	C	TYR	A	156	45.351	34.041	54.691	1.00	6.48	6
ATOM	1269	O	TYR	A	156	44.907	32.991	55.146	1.00	6.37	8
ATOM	1270	N	HIS	A	157	44.751	34.691	53.719	1.00	5.96	7
ATOM	1271	CA	HIS	A	157	43.567	34.321	53.016	1.00	5.71	6
ATOM	1272	CB	HIS	A	157	42.768	35.566	52.552	1.00	5.00	6

ATOM	1273	CG	HIS	A	157	42.236	36.398	53.732	1.00	5.00	6
ATOM	1274	CD2	HIS	A	157	41.620	36.018	54.866	1.00	5.00	6
ATOM	1275	ND1	HIS	A	157	42.426	37.765	53.793	1.00	5.10	7
ATOM	1276	CE1	HIS	A	157	41.880	38.216	54.935	1.00	6.49	6
ATOM	1277	NE2	HIS	A	157	41.398	37.147	55.588	1.00	5.12	7
ATOM	1278	C	HIS	A	157	43.896	33.473	51.753	1.00	5.75	6
ATOM	1279	O	HIS	A	157	43.028	33.056	50.978	1.00	5.63	8
ATOM	1280	N	PHE	A	158	45.182	33.311	51.471	1.00	5.60	7
ATOM	1281	CA	PHE	A	158	45.722	32.597	50.312	1.00	5.84	6
ATOM	1282	CB	PHE	A	158	46.578	33.527	49.412	1.00	5.00	6
ATOM	1283	CG	PHE	A	158	45.867	34.784	48.992	1.00	5.00	6
ATOM	1284	CD1	PHE	A	158	46.099	35.994	49.658	1.00	5.00	6
ATOM	1285	CD2	PHE	A	158	44.972	34.788	47.942	1.00	5.00	6
ATOM	1286	CE1	PHE	A	158	45.418	37.147	49.286	1.00	6.00	6
ATOM	1287	CE2	PHE	A	158	44.300	35.931	47.568	1.00	5.36	6
ATOM	1288	CZ	PHE	A	158	44.494	37.129	48.230	1.00	5.65	6
ATOM	1289	C	PHE	A	158	46.580	31.365	50.692	1.00	5.86	6
ATOM	1290	O	PHE	A	158	47.192	31.311	51.800	1.00	5.98	8
ATOM	1291	N	ASP	A	159	46.638	30.354	49.804	1.00	5.59	7
ATOM	1292	CA	ASP	A	159	47.461	29.211	50.022	1.00	5.30	6
ATOM	1293	CB	ASP	A	159	46.924	27.979	49.262	1.00	5.00	6
ATOM	1294	CG	ASP	A	159	45.876	27.378	50.090	1.00	5.58	6
ATOM	1295	OD1	ASP	A	159	45.988	27.501	51.360	1.00	8.12	8
ATOM	1296	OD2	ASP	A	159	44.852	26.813	49.700	1.00	5.00	8
ATOM	1297	C	ASP	A	159	48.876	29.377	49.478	1.00	5.70	6
ATOM	1298	O	ASP	A	159	49.808	28.719	49.999	1.00	6.04	8
ATOM	1299	N	GLY	A	160	49.083	30.164	48.444	1.00	5.67	7
ATOM	1300	CA	GLY	A	160	50.438	30.251	47.914	1.00	6.24	6
ATOM	1301	C	GLY	A	160	50.472	31.296	46.798	1.00	6.82	6
ATOM	1302	O	GLY	A	160	49.389	31.807	46.477	1.00	6.74	8
ATOM	1303	N	ALA	A	161	51.622	31.520	46.224	1.00	7.20	7
ATOM	1304	CA	ALA	A	161	51.756	32.488	45.174	1.00	8.08	6
ATOM	1305	CB	ALA	A	161	52.023	33.869	45.775	1.00	8.88	6
ATOM	1306	C	ALA	A	161	52.933	32.083	44.297	1.00	9.05	6
ATOM	1307	O	ALA	A	161	53.582	31.055	44.591	1.00	8.86	8
ATOM	1308	N	ASP	A	162	53.158	32.846	43.215	1.00	10.00	7
ATOM	1309	CA	ASP	A	162	54.278	32.418	42.372	1.00	11.36	6
ATOM	1310	CB	ASP	A	162	53.786	32.031	40.983	1.00	15.10	6
ATOM	1311	CG	ASP	A	162	53.111	33.242	40.352	1.00	19.35	6
ATOM	1312	OD1	ASP	A	162	52.930	34.331	40.947	1.00	19.47	8
ATOM	1313	OD2	ASP	A	162	52.725	32.956	39.169	1.00	22.93	8
ATOM	1314	C	ASP	A	162	55.381	33.455	42.149	1.00	11.95	6
ATOM	1315	O	ASP	A	162	56.107	33.336	41.131	1.00	12.10	8
ATOM	1316	N	TRP	A	163	55.489	34.435	43.048	1.00	12.03	7
ATOM	1317	CA	TRP	A	163	56.533	35.418	42.793	1.00	12.34	6
ATOM	1318	CB	TRP	A	163	55.954	36.485	41.881	1.00	12.40	6
ATOM	1319	CG	TRP	A	163	56.925	37.600	41.631	1.00	13.20	6
ATOM	1320	CD2	TRP	A	163	58.014	37.602	40.715	1.00	14.18	6
ATOM	1321	CE2	TRP	A	163	58.646	38.869	40.826	1.00	15.32	6
ATOM	1322	CE3	TRP	A	163	58.520	36.667	39.803	1.00	14.71	6
ATOM	1323	CD1	TRP	A	163	56.950	38.813	42.245	1.00	13.62	6
ATOM	1324	NE1	TRP	A	163	57.980	39.589	41.774	1.00	13.74	7
ATOM	1325	CZ2	TRP	A	163	59.757	39.243	40.036	1.00	16.07	6
ATOM	1326	CZ3	TRP	A	163	59.639	37.017	39.046	1.00	14.61	6
ATOM	1327	CH2	TRP	A	163	60.210	38.279	39.139	1.00	16.01	6
ATOM	1328	C	TRP	A	163	57.008	35.969	44.102	1.00	12.82	6
ATOM	1329	O	TRP	A	163	56.225	36.180	45.012	1.00	12.72	8
ATOM	1330	N	ASP	A	164	58.298	36.130	44.243	1.00	13.51	7
ATOM	1331	CA	ASP	A	164	58.961	36.679	45.420	1.00	14.00	6
ATOM	1332	CB	ASP	A	164	60.073	35.796	45.937	1.00	13.67	6
ATOM	1333	CG	ASP	A	164	60.891	36.513	47.003	1.00	14.44	6
ATOM	1334	OD1	ASP	A	164	60.392	37.464	47.682	1.00	14.14	8
ATOM	1335	OD2	ASP	A	164	62.070	36.096	47.155	1.00	15.41	8
ATOM	1336	C	ASP	A	164	59.560	38.004	44.913	1.00	14.37	6
ATOM	1337	O	ASP	A	164	60.491	37.969	44.125	1.00	14.14	8
ATOM	1338	N	GLU	A	165	59.024	39.109	45.390	1.00	14.96	7
ATOM	1339	CA	GLU	A	165	59.449	40.429	44.953	1.00	15.64	6
ATOM	1340	CB	GLU	A	165	58.453	41.456	45.446	1.00	15.08	6
ATOM	1341	CG	GLU	A	165	58.724	42.887	45.070	1.00	16.95	6
ATOM	1342	CD	GLU	A	165	58.627	43.079	43.584	1.00	18.88	6
ATOM	1343	OE1	GLU	A	165	59.126	44.095	43.075	1.00	22.59	8
ATOM	1344	OE2	GLU	A	165	58.071	42.288	42.822	1.00	19.30	8
ATOM	1345	C	GLU	A	165	60.843	40.736	45.498	1.00	16.33	6
ATOM	1346	O	GLU	A	165	61.504	41.590	44.951	1.00	16.30	8
ATOM	1347	N	SER	A	166	61.227	40.104	46.593	1.00	16.71	7
ATOM	1348	CA	SER	A	166	62.499	40.241	47.255	1.00	17.23	6
ATOM	1349	CB	SER	A	166	62.471	39.215	48.415	1.00	17.88	6
ATOM	1350	OG	SER	A	166	63.157	39.838	49.443	1.00	21.31	8
ATOM	1351	C	SER	A	166	63.694	39.857	46.363	1.00	17.59	6
ATOM	1352	O	SER	A	166	64.511	40.670	45.931	1.00	17.48	8
ATOM	1353	N	ARG	A	167	63.756	38.534	46.062	1.00	17.53	7
ATOM	1354	CA	ARG	A	167	64.754	37.962	45.202	1.00	17.50	6
ATOM	1355	CB	ARG	A	167	64.972	36.483	45.538	1.00	18.49	6
ATOM	1356	CG	ARG	A	167	65.372	36.319	46.984	1.00	19.67	6
ATOM	1357	CD	ARG	A	167	65.413	34.810	47.294	1.00	22.11	6
ATOM	1358	NE	ARG	A	167	65.554	34.699	48.736	1.00	24.69	7
ATOM	1359	CZ	ARG	A	167	64.638	35.047	49.658	1.00	27.34	6
ATOM	1360	NH1	ARG	A	167	63.420	35.550	49.443	1.00	24.66	7
ATOM	1361	NH2	ARG	A	167	65.027	34.853	50.954	1.00	28.95	7
ATOM	1362	C	ARG	A	167	64.344	38.047	43.729	1.00	17.36	6
ATOM	1363	O	ARG	A	167	65.179	37.757	42.880	1.00	17.29	8
ATOM	1364	N	LYS	A	168	63.124	38.406	43.386	1.00	17.25	7
ATOM	1365	CA	LYS	A	168	62.636	38.491	42.048	1.00	17.27	6
ATOM	1366	CB	LYS	A	168	63.318	39.579	41.203	1.00	20.36	6
ATOM	1367	CG	LYS	A	168	62.818	40.920	41.752	1.00	23.95	6
ATOM	1368	CD	LYS	A	168	63.605	42.120	41.269	1.00	26.67	6
ATOM	1369	CE	LYS	A	168	62.855	43.415	41.686	1.00	28.90	6
ATOM	1370	NZ	LYS	A	168	62.830	43.494	43.201	1.00	30.66	7
ATOM	1371	C	LYS	A	168	62.766	37.148	41.332	1.00	17.23	6
ATOM	1372	O	LYS	A	168	63.337	37.062	40.229	1.00	17.13	8
ATOM	1373	N	ILE	A	169	62.203	36.106	41.956	1.00	16.95	7
ATOM	1374	CA	ILE	A	169	62.199	34.766	41.380	1.00	16.59	6
ATOM	1375	CB	ILE	A	169	63.086	33.751	42.115	1.00	17.17	6
ATOM	1376	CG2	ILE	A	169	64.599	34.139	42.040	1.00	16.91	6
ATOM	1377	CG1	ILE	A	169	62.641	33.597	43.557	1.00	17.77	6
ATOM	1378	CD1	ILE	A	169	63.595	32.811	44.434	1.00	18.17	6

ATOM	1379	C	ILE	A	169	60.748	34.265	41.354	1.00	16.43	6
ATOM	1380	O	ILE	A	169	59.894	34.602	42.175	1.00	15.97	8
ATOM	1381	N	SER	A	170	60.458	33.469	40.342	1.00	16.39	7
ATOM	1382	CA	SER	A	170	59.209	32.808	40.120	1.00	16.32	6
ATOM	1383	CB	SER	A	170	58.830	32.767	38.642	1.00	18.20	6
ATOM	1384	OG	SER	A	170	57.519	32.181	38.607	1.00	22.81	8
ATOM	1385	C	SER	A	170	59.306	31.335	40.518	1.00	16.18	6
ATOM	1386	O	SER	A	170	60.106	30.599	39.908	1.00	16.17	8
ATOM	1387	N	ARG	A	171	58.531	30.882	41.508	1.00	15.84	7
ATOM	1388	CA	ARG	A	171	58.504	29.492	41.954	1.00	15.28	6
ATOM	1389	CB	ARG	A	171	59.448	29.168	43.104	1.00	17.32	6
ATOM	1390	CG	ARG	A	171	60.894	29.497	43.152	1.00	19.88	6
ATOM	1391	CD	ARG	A	171	61.825	28.448	42.555	1.00	23.48	6
ATOM	1392	NE	ARG	A	171	63.204	28.981	42.466	1.00	27.05	7
ATOM	1393	CZ	ARG	A	171	63.661	29.577	41.358	1.00	29.43	6
ATOM	1394	NH1	ARG	A	171	62.909	29.718	40.256	1.00	30.87	7
ATOM	1395	NH2	ARG	A	171	64.884	30.070	41.191	1.00	30.59	7
ATOM	1396	C	ARG	A	171	57.052	29.164	42.380	1.00	14.63	6
ATOM	1397	O	ARG	A	171	56.203	30.055	42.313	1.00	14.71	8
ATOM	1398	N	ILE	A	172	56.737	27.949	42.824	1.00	13.80	7
ATOM	1399	CA	ILE	A	172	55.389	27.671	43.336	1.00	13.02	6
ATOM	1400	CB	ILE	A	172	54.752	26.357	42.862	1.00	11.93	6
ATOM	1401	CG2	ILE	A	172	53.502	26.058	43.656	1.00	11.06	6
ATOM	1402	CG1	ILE	A	172	54.360	26.386	41.354	1.00	11.59	6
ATOM	1403	CD1	ILE	A	172	53.920	25.010	40.927	1.00	12.67	6
ATOM	1404	C	ILE	A	172	55.639	27.730	44.867	1.00	12.55	6
ATOM	1405	O	ILE	A	172	56.218	26.808	45.469	1.00	12.52	8
ATOM	1406	N	PHE	A	173	55.290	28.812	45.529	1.00	11.95	7
ATOM	1407	CA	PHE	A	173	55.464	28.982	46.956	1.00	11.52	6
ATOM	1408	CB	PHE	A	173	55.813	30.424	47.326	1.00	8.63	6
ATOM	1409	CG	PHE	A	173	57.088	30.932	46.719	1.00	8.19	6
ATOM	1410	CD1	PHE	A	173	57.085	31.845	45.697	1.00	6.97	6
ATOM	1411	CD2	PHE	A	173	58.313	30.470	47.211	1.00	8.07	6
ATOM	1412	CE1	PHE	A	173	58.277	32.307	45.123	1.00	8.69	6
ATOM	1413	CE2	PHE	A	173	59.512	30.949	46.686	1.00	8.72	6
ATOM	1414	CZ	PHE	A	173	59.484	31.844	45.607	1.00	7.75	6
ATOM	1415	C	PHE	A	173	54.189	28.583	47.688	1.00	11.50	6
ATOM	1416	O	PHE	A	173	53.109	29.085	47.372	1.00	11.79	8
ATOM	1417	N	LYS	A	174	54.257	27.696	48.657	1.00	11.28	7
ATOM	1418	CA	LYS	A	174	53.185	27.303	49.524	1.00	11.02	6
ATOM	1419	CB	LYS	A	174	53.268	25.849	49.981	1.00	7.54	6
ATOM	1420	CG	LYS	A	174	52.045	25.443	50.770	1.00	6.03	6
ATOM	1421	CD	LYS	A	174	51.880	23.947	50.993	1.00	5.90	6
ATOM	1422	CE	LYS	A	174	53.109	23.439	51.713	1.00	6.00	6
ATOM	1423	NZ	LYS	A	174	52.991	22.034	52.176	1.00	5.20	7
ATOM	1424	C	LYS	A	174	53.313	28.195	50.787	1.00	11.19	6
ATOM	1425	O	LYS	A	174	54.402	28.117	51.406	1.00	11.32	8
ATOM	1426	N	PHE	A	175	52.357	28.950	51.264	1.00	11.10	7
ATOM	1427	CA	PHE	A	175	52.555	29.759	52.486	1.00	11.23	6
ATOM	1428	CB	PHE	A	175	51.440	30.845	52.516	1.00	9.58	6
ATOM	1429	CG	PHE	A	175	51.497	31.920	51.427	1.00	9.11	6
ATOM	1430	CD1	PHE	A	175	50.410	32.806	51.283	1.00	8.73	6
ATOM	1431	CD2	PHE	A	175	52.569	32.097	50.557	1.00	7.13	6
ATOM	1432	CE1	PHE	A	175	50.443	33.823	50.320	1.00	7.64	6
ATOM	1433	CE2	PHE	A	175	52.585	33.103	49.614	1.00	6.81	6
ATOM	1434	CZ	PHE	A	175	51.517	33.983	49.476	1.00	7.21	6
ATOM	1435	C	PHE	A	175	52.567	28.942	53.770	1.00	11.49	6
ATOM	1436	O	PHE	A	175	51.868	27.912	53.875	1.00	11.44	8
ATOM	1437	N	ARG	A	176	53.288	29.352	54.813	1.00	11.77	7
ATOM	1438	CA	ARG	A	176	53.328	28.725	56.129	1.00	12.20	6
ATOM	1439	CB	ARG	A	176	54.684	28.802	56.775	1.00	13.53	6
ATOM	1440	CG	ARG	A	176	55.768	27.776	56.372	1.00	14.88	6
ATOM	1441	CD	ARG	A	176	55.188	26.438	56.823	1.00	15.37	6
ATOM	1442	NE	ARG	A	176	56.133	25.355	56.737	1.00	15.69	7
ATOM	1443	CZ	ARG	A	176	56.118	24.277	55.962	1.00	16.02	6
ATOM	1444	NH1	ARG	A	176	55.150	24.037	.55.065	1.00	16.35	7
ATOM	1445	NH2	ARG	A	176	57.151	23.430	56.062	1.00	16.02	7
ATOM	1446	C	ARG	A	176	52.330	29.526	56.994	1.00	12.82	6
ATOM	1447	O	ARG	A	176	52.303	30.774	56.778	1.00	12.92	8
ATOM	1448	N	GLY	A	177	51.560	28.911	57.850	1.00	13.07	7
ATOM	1449	CA	GLY	A	177	50.590	29.656	58.637	1.00	13.84	6
ATOM	1450	C	GLY	A	177	49.736	28.715	59.449	1.00	14.51	6
ATOM	1451	O	GLY	A	177	50.056	27.482	59.489	1.00	15.11	8
ATOM	1452	N	GLU	A	178	48.649	29.125	60.069	1.00	14.47	7
ATOM	1453	CA	GLU	A	178	47.810	28.222	60.859	1.00	14.86	6
ATOM	1454	CB	GLU	A	178	46.912	29.021	61.833	1.00	15.74	6
ATOM	1455	CG	GLU	A	178	47.575	29.715	63.000	1.00	16.47	6
ATOM	1456	CD	GLU	A	178	48.458	28.762	63.819	1.00	18.26	6
ATOM	1457	OE1	GLU	A	178	48.216	27.504	63.969	1.00	19.50	8
ATOM	1458	OE2	GLU	A	178	49.488	29.266	64.326	1.00	16.85	8
ATOM	1459	C	GLU	A	178	46.961	27.310	59.957	1.00	15.02	6
ATOM	1460	O	GLU	A	178	46.138	27.801	59.151	1.00	15.35	8
ATOM	1461	N	GLY	A	179	47.148	26.015	60.032	1.00	14.81	7
ATOM	1462	CA	GLY	A	179	46.450	25.042	59.221	1.00	14.68	6
ATOM	1463	C	GLY	A	179	46.692	25.221	57.702	1.00	14.28	6
ATOM	1464	O	GLY	A	179	45.709	24.906	56.979	1.00	14.54	8
ATOM	1465	N	LYS	A	180	47.854	25.708	57.243	1.00	13.43	7
ATOM	1466	CA	LYS	A	180	48.022	25.959	55.824	1.00	12.55	6
ATOM	1467	CB	LYS	A	180	49.163	26.955	55.631	1.00	11.48	6
ATOM	1468	CG	LYS	A	180	48.825	28.409	55.816	1.00	11.89	6
ATOM	1469	CD	LYS	A	180	47.710	28.914	54.938	1.00	9.28	6
ATOM	1470	CE	LYS	A	180	47.355	30.371	55.116	1.00	9.37	6
ATOM	1471	NZ	LYS	A	180	46.097	30.683	54.339	1.00	9.60	7
ATOM	1472	C	LYS	A	180	48.271	24.676	55.037	1.00	12.15	6
ATOM	1473	O	LYS	A	180	49.150	23.919	55.465	1.00	12.30	8
ATOM	1474	N	ALA	A	181	47.571	24.402	53.925	1.00	11.19	7
ATOM	1475	CA	ALA	A	181	47.792	23.208	53.139	1.00	10.23	6
ATOM	1476	CB	ALA	A	181	47.183	21.975	53.825	1.00	8.27	6
ATOM	1477	C	ALA	A	181	47.120	23.287	51.761	1.00	9.57	6
ATOM	1478	O	ALA	A	181	46.125	23.952	51.862	1.00	8.95	8
ATOM	1479	N	TRP	A	182	47.457	22.762	50.604	1.00	8.86	7
ATOM	1480	CA	TRP	A	182	46.604	22.929	49.465	1.00	8.54	6
ATOM	1481	CB	TRP	A	182	47.232	22.145	48.309	1.00	6.73	6
ATOM	1482	CG	TRP	A	182	48.624	22.609	47.966	1.00	5.79	6
ATOM	1483	CD2	TRP	A	182	49.003	23.922	47.558	1.00	5.00	6
ATOM	1484	CE2	TRP	A	182	50.388	23.887	47.314	1.00	5.13	6

SUBSTITUTE SHEET (RULE 26)

Appendix 1

ATOM	1485	CE3	TRP	A	182	48.278	25.127	47.361	1.00	5.00	6
ATOM	1486	CD1	TRP	A	182	49.768	21.861	48.002	1.00	5.63	6
ATOM	1487	NE1	TRP	A	182	50.860	22.616	47.616	1.00	5.04	7
ATOM	1488	CZ2	TRP	A	182	51.110	25.022	46.895	1.00	5.00	6
ATOM	1489	CZ3	TRP	A	182	48.966	26.236	46.927	1.00	5.00	6
ATOM	1490	CH2	TRP	A	182	50.376	26.186	46.723	1.00	5.00	6
ATOM	1491	C	TRP	A	182	45.218	22.348	49.787	1.00	8.52	6
ATOM	1492	O	TRP	A	182	45.029	21.400	50.552	1.00	8.24	8
ATOM	1493	N	ASP	A	183	44.187	22.939	49.183	1.00	8.61	7
ATOM	1494	CA	ASP	A	183	42.814	22.546	49.339	1.00	8.57	6
ATOM	1495	CB	ASP	A	183	41.746	23.407	48.669	1.00	7.64	6
ATOM	1496	CG	ASP	A	183	41.829	24.846	49.207	1.00	7.97	6
ATOM	1497	OD1	ASP	A	183	42.136	25.011	50.384	1.00	5.19	8
ATOM	1498	OD2	ASP	A	183	41.604	25.903	48.623	1.00	7.20	8
ATOM	1499	C	ASP	A	183	42.678	21.163	48.661	1.00	8.68	6
ATOM	1500	O	ASP	A	183	43.392	20.764	47.757	1.00	8.29	8
ATOM	1501	N	TRP	A	184	41.655	20.526	49.221	1.00	8.85	7
ATOM	1502	CA	TRP	A	184	41.337	19.214	48.816	1.00	9.31	6
ATOM	1503	CB	TRP	A	184	42.068	18.015	49.485	1.00	9.16	6
ATOM	1504	CG	TRP	A	184	41.858	16.719	48.814	1.00	9.24	6
ATOM	1505	CD2	TRP	A	184	42.391	16.211	47.580	1.00	9.64	6
ATOM	1506	CE2	TRP	A	184	41.870	14.896	47.384	1.00	9.60	6
ATOM	1507	CE3	TRP	A	184	43.240	16.730	46.594	1.00	8.61	6
ATOM	1508	CD1	TRP	A	184	41.009	15.713	49.300	1.00	10.78	6
ATOM	1509	NE1	TRP	A	184	41.019	14.620	48.426	1.00	9.86	7
ATOM	1510	CZ2	TRP	A	184	42.149	14.151	46.250	1.00	9.85	6
ATOM	1511	CZ3	TRP	A	184	43.547	15.968	45.479	1.00	9.71	6
ATOM	1512	CH2	TRP	A	184	43.008	14.693	45.314	1.00	9.96	6
ATOM	1513	C	TRP	A	184	39.766	18.960	48.936	1.00	9.70	6
ATOM	1514	O	TRP	A	184	39.093	19.322	49.789	1.00	10.01	8
ATOM	1515	N	GLU	A	185	39.594	18.432	47.785	1.00	9.88	7
ATOM	1516	CA	GLU	A	185	39.263	17.724	46.655	1.00	9.32	6
ATOM	1517	CB	GLU	A	185	38.201	16.707	46.321	1.00	11.19	6
ATOM	1518	CG	GLU	A	185	38.829	15.901	45.132	1.00	11.41	6
ATOM	1519	CD	GLU	A	185	38.070	14.631	44.814	1.00	13.77	6
ATOM	1520	OE1	GLU	A	185	37.147	14.228	45.559	1.00	14.04	8
ATOM	1521	OE2	GLU	A	185	38.349	14.001	43.768	1.00	14.41	8
ATOM	1522	C	GLU	A	185	39.394	18.759	45.479	1.00	8.78	6
ATOM	1523	O	GLU	A	185	38.591	19.636	45.294	1.00	8.92	8
ATOM	1524	N	VAL	A	186	40.502	18.566	44.792	1.00	8.34	7
ATOM	1525	CA	VAL	A	186	40.810	19.326	43.583	1.00	8.33	6
ATOM	1526	CB	VAL	A	186	41.807	20.506	43.735	1.00	8.32	6
ATOM	1527	CG1	VAL	A	186	41.196	21.617	44.616	1.00	7.05	6
ATOM	1528	CG2	VAL	A	186	43.173	20.110	44.308	1.00	5.20	6
ATOM	1529	C	VAL	A	186	41.364	18.291	42.578	1.00	8.42	6
ATOM	1530	O	VAL	A	186	41.505	17.111	42.956	1.00	8.25	8
ATOM	1531	N	SER	A	187	41.735	18.666	41.367	1.00	8.40	7
ATOM	1532	CA	SER	A	187	42.313	17.723	40.445	1.00	8.96	6
ATOM	1533	CB	SER	A	187	42.664	18.422	39.113	1.00	8.95	6
ATOM	1534	OG	SER	A	187	43.472	17.537	38.328	1.00	8.65	8
ATOM	1535	C	SER	A	187	43.603	17.153	41.060	1.00	9.46	6
ATOM	1536	O	SER	A	187	44.375	17.887	41.684	1.00	9.28	8
ATOM	1537	N	SER	A	188	43.908	15.846	40.823	1.00	9.77	7
ATOM	1538	CA	SER	A	188	45.109	15.208	41.353	1.00	9.72	6
ATOM	1539	CB	SER	A	188	44.906	13.770	41.859	1.00	10.83	6
ATOM	1540	OG	SER	A	188	44.547	12.983	40.714	1.00	12.11	8
ATOM	1541	C	SER	A	188	46.215	15.213	40.288	1.00	9.72	6
ATOM	1542	O	SER	A	188	47.239	14.540	40.529	1.00	9.62	8
ATOM	1543	N	GLU	A	189	46.009	15.968	39.192	1.00	9.48	7
ATOM	1544	CA	GLU	A	189	47.091	16.143	38.252	1.00	9.58	6
ATOM	1545	CB	GLU	A	189	46.761	17.025	37.029	1.00	12.65	6
ATOM	1546	CG	GLU	A	189	45.655	16.361	36.202	1.00	14.93	6
ATOM	1547	CD	GLU	A	189	44.958	17.419	35.359	1.00	16.59	6
ATOM	1548	OE1	GLU	A	189	44.060	18.118	35.868	1.00	16.06	8
ATOM	1549	OE2	GLU	A	189	45.364	17.496	34.187	1.00	19.90	8
ATOM	1550	C	GLU	A	189	48.208	16.888	38.998	1.00	9.38	6
ATOM	1551	O	GLU	A	189	47.948	17.852	39.783	1.00	9.35	8
ATOM	1552	N	ASN	A	190	49.447	16.512	38.785	1.00	9.02	7
ATOM	1553	CA	ASN	A	190	50.591	17.137	39.437	1.00	8.98	6
ATOM	1554	CB	ASN	A	190	50.708	18.629	39.139	1.00	11.63	6
ATOM	1555	CG	ASN	A	190	50.842	19.067	37.714	1.00	13.22	6
ATOM	1556	OD1	ASN	A	190	51.553	18.489	36.913	1.00	13.96	8
ATOM	1557	ND2	ASN	A	190	50.145	20.093	37.234	1.00	14.84	7
ATOM	1558	C	ASN	A	190	50.548	16.928	40.959	1.00	8.84	6
ATOM	1559	O	ASN	A	190	51.020	17.773	41.750	1.00	9.06	8
ATOM	1560	N	GLY	A	191	49.949	15.854	41.439	1.00	8.36	7
ATOM	1561	CA	GLY	A	191	49.772	15.467	42.809	1.00	7.95	6
ATOM	1562	C	GLY	A	191	48.597	16.148	43.430	1.00	7.74	6
ATOM	1563	O	GLY	A	191	47.747	15.586	44.065	1.00	7.89	8
ATOM	1564	N	ASN	A	192	48.537	17.450	43.284	1.00	7.66	7
ATOM	1565	CA	ASN	A	192	47.472	18.353	43.732	1.00	7.21	6
ATOM	1566	CB	ASN	A	192	47.596	18.649	45.227	1.00	8.14	6
ATOM	1567	CG	ASN	A	192	46.628	19.665	45.785	1.00	7.93	6
ATOM	1568	OD1	ASN	A	192	46.584	20.794	45.287	1.00	8.55	8
ATOM	1569	ND2	ASN	A	192	45.839	19.388	46.805	1.00	7.17	7
ATOM	1570	C	ASN	A	192	47.572	19.615	42.863	1.00	6.90	6
ATOM	1571	O	ASN	A	192	48.574	20.328	42.910	1.00	6.69	8
ATOM	1572	N	TYR	A	193	46.517	19.881	42.099	1.00	6.77	7
ATOM	1573	CA	TYR	A	193	46.405	20.986	41.210	1.00	7.00	6
ATOM	1574	CB	TYR	A	193	45.725	20.535	39.867	1.00	7.52	6
ATOM	1575	CG	TYR	A	193	46.348	21.143	38.659	1.00	8.30	6
ATOM	1576	CD1	TYR	A	193	46.218	20.596	37.385	1.00	8.97	6
ATOM	1577	CE1	TYR	A	193	46.841	21.202	36.283	1.00	9.17	6
ATOM	1578	CD2	TYR	A	193	47.096	22.301	38.738	1.00	8.68	6
ATOM	1579	CE2	TYR	A	193	47.695	22.928	37.673	1.00	9.08	6
ATOM	1580	CZ	TYR	A	193	47.564	22.343	36.424	1.00	9.29	6
ATOM	1581	OH	TYR	A	193	48.177	22.966	35.361	1.00	9.62	8
ATOM	1582	C	TYR	A	193	45.646	22.201	41.776	1.00	6.92	6
ATOM	1583	O	TYR	A	193	45.034	22.979	41.061	1.00	6.78	8
ATOM	1584	N	ASP	A	194	45.662	22.448	43.066	1.00	6.98	7
ATOM	1585	CA	ASP	A	194	45.102	23.587	43.773	1.00	6.81	6
ATOM	1586	CB	ASP	A	194	45.338	23.579	45.279	1.00	7.26	6
ATOM	1587	CG	ASP	A	194	44.586	24.609	46.082	1.00	8.65	6
ATOM	1588	OD1	ASP	A	194	43.590	25.127	45.523	1.00	9.18	8
ATOM	1589	OD2	ASP	A	194	44.730	24.922	47.280	1.00	8.87	8
ATOM	1590	C	ASP	A	194	45.815	24.809	43.156	1.00	6.63	6

ATOM	1591	O	ASP	A	194	45.143	25.681	42.616	1.00	6.42	8
ATOM	1592	N	TYR	A	195	47.129	24.919	43.145	1.00	6.43	7
ATOM	1593	CA	TYR	A	195	47.781	26.059	42.596	1.00	6.19	6
ATOM	1594	CB	TYR	A	195	49.261	26.101	43.153	1.00	5.52	6
ATOM	1595	CG	TYR	A	195	49.722	27.472	42.821	1.00	5.15	6
ATOM	1596	CD1	TYR	A	195	49.314	28.569	43.582	1.00	5.28	6
ATOM	1597	CE1	TYR	A	195	49.676	29.862	43.186	1.00	5.27	6
ATOM	1598	CD2	TYR	A	195	50.456	27.686	41.665	1.00	5.05	6
ATOM	1599	CE2	TYR	A	195	50.809	28.972	41.246	1.00	5.06	6
ATOM	1600	CZ	TYR	A	195	50.386	30.053	42.030	1.00	5.27	6
ATOM	1601	OH	TYR	A	195	50.742	31.310	41.636	1.00	5.27	8
ATOM	1602	C	TYR	A	195	47.730	26.123	41.082	1.00	6.73	6
ATOM	1603	O	TYR	A	195	48.128	25.186	40.392	1.00	6.74	8
ATOM	1604	N	LEU	A	196	47.329	27.323	40.580	1.00	7.17	7
ATOM	1605	CA	LEU	A	196	47.346	27.572	39.148	1.00	7.71	6
ATOM	1606	CB	LEU	A	196	45.962	27.721	38.510	1.00	6.89	6
ATOM	1607	CG	LEU	A	196	45.988	28.100	37.020	1.00	8.29	6
ATOM	1608	CD1	LEU	A	196	46.520	26.975	36.126	1.00	6.67	6
ATOM	1609	CD2	LEU	A	196	44.578	28.516	36.621	1.00	7.69	6
ATOM	1610	C	LEU	A	196	48.181	28.816	38.807	1.00	7.86	6
ATOM	1611	O	LEU	A	196	49.162	28.671	38.073	1.00	7.98	8
ATOM	1612	N	MET	A	197	47.861	29.990	39.319	1.00	7.94	7
ATOM	1613	CA	MET	A	197	48.577	31.228	39.029	1.00	8.00	6
ATOM	1614	CB	MET	A	197	48.230	31.699	37.613	1.00	11.16	6
ATOM	1615	CG	MET	A	197	46.758	32.064	37.445	1.00	15.62	6
ATOM	1616	SD	MET	A	197	46.223	32.419	35.732	1.00	22.83	16
ATOM	1617	CE	MET	A	197	47.695	33.237	35.117	1.00	21.60	6
ATOM	1618	C	MET	A	197	48.157	32.310	40.032	1.00	7.71	6
ATOM	1619	O	MET	A	197	47.200	32.162	40.792	1.00	7.22	8
ATOM	1620	N	TYR	A	198	48.875	33.421	39.997	1.00	7.95	7
ATOM	1621	CA	TYR	A	198	48.725	34.595	40.849	1.00	8.22	6
ATOM	1622	CB	TYR	A	198	47.512	35.420	40.476	1.00	9.23	6
ATOM	1623	CG	TYR	A	198	47.601	35.991	39.081	1.00	10.99	6
ATOM	1624	CD1	TYR	A	198	46.600	35.690	38.145	1.00	11.90	6
ATOM	1625	CE1	TYR	A	198	46.655	36.230	36.875	1.00	12.83	6
ATOM	1626	CD2	TYR	A	198	48.664	36.817	38.741	1.00	11.91	6
ATOM	1627	CE2	TYR	A	198	48.745	37.364	37.443	1.00	12.82	6
ATOM	1628	CZ	TYR	A	198	47.741	37.045	36.538	1.00	13.43	6
ATOM	1629	OH	TYR	A	198	47.797	37.589	35.261	1.00	14.37	8
ATOM	1630	C	TYR	A	198	48.629	34.167	42.312	1.00	7.86	6
ATOM	1631	O	TYR	A	198	49.362	33.257	42.693	1.00	7.88	8
ATOM	1632	N	ALA	A	199	47.769	34.787	43.117	1.00	7.31	7
ATOM	1633	CA	ALA	A	199	47.563	34.481	44.537	1.00	6.22	6
ATOM	1634	CB	ALA	A	199	47.321	35.747	45.359	1.00	6.68	6
ATOM	1635	C	ALA	A	199	46.389	33.523	44.687	1.00	5.38	6
ATOM	1636	O	ALA	A	199	45.255	33.918	44.370	1.00	5.00	8
ATOM	1637	N	ASP	A	200	46.702	32.319	45.148	1.00	5.09	7
ATOM	1638	CA	ASP	A	200	45.748	31.224	45.295	1.00	5.00	6
ATOM	1639	CB	ASP	A	200	46.567	29.901	45.278	1.00	5.25	6
ATOM	1640	CG	ASP	A	200	45.495	28.798	45.141	1.00	6.80	6
ATOM	1641	OD1	ASP	A	200	44.912	28.830	44.024	1.00	6.41	8
ATOM	1642	OD2	ASP	A	200	45.139	27.965	46.011	1.00	6.48	8
ATOM	1643	C	ASP	A	200	44.879	31.313	46.526	1.00	5.00	6
ATOM	1644	O	ASP	A	200	45.308	31.320	47.681	1.00	5.31	8
ATOM	1645	N	VAL	A	201	43.567	31.445	46.359	1.00	5.00	7
ATOM	1646	CA	VAL	A	201	42.610	31.603	47.446	1.00	5.00	6
ATOM	1647	CB	VAL	A	201	41.215	31.999	46.911	1.00	5.00	6
ATOM	1648	CG1	VAL	A	201	40.249	32.082	48.070	1.00	5.00	6
ATOM	1649	CG2	VAL	A	201	41.205	33.336	46.136	1.00	5.00	6
ATOM	1650	C	VAL	A	201	42.542	30.306	48.243	1.00	5.00	6
ATOM	1651	O	VAL	A	201	42.387	29.199	47.732	1.00	5.00	8
ATOM	1652	N	ASP	A	202	42.605	30.491	49.571	1.00	5.00	7
ATOM	1653	CA	ASP	A	202	42.519	29.430	50.556	1.00	5.00	6
ATOM	1654	CB	ASP	A	202	43.337	29.878	51.801	1.00	5.82	6
ATOM	1655	CG	ASP	A	202	43.437	28.834	52.876	1.00	6.39	6
ATOM	1656	OD1	ASP	A	202	42.805	27.761	52.605	1.00	5.70	8
ATOM	1657	OD2	ASP	A	202	44.017	28.814	53.965	1.00	6.27	8
ATOM	1658	C	ASP	A	202	41.060	29.141	50.949	1.00	5.00	6
ATOM	1659	O	ASP	A	202	40.518	29.810	51.838	1.00	5.00	8
ATOM	1660	N	TYR	A	203	40.418	28.138	50.330	1.00	5.00	7
ATOM	1661	CA	TYR	A	203	39.019	27.825	50.636	1.00	5.09	6
ATOM	1662	CB	TYR	A	203	38.234	27.239	49.448	1.00	5.00	6
ATOM	1663	CG	TYR	A	203	38.008	28.366	48.426	1.00	5.00	6
ATOM	1664	CD1	TYR	A	203	38.653	28.457	47.236	1.00	5.00	6
ATOM	1665	CE1	TYR	A	203	38.449	29.510	46.379	1.00	5.00	6
ATOM	1666	CD2	TYR	A	203	37.124	29.393	48.827	1.00	5.05	6
ATOM	1667	CE2	TYR	A	203	36.914	30.493	47.963	1.00	5.07	6
ATOM	1668	CZ	TYR	A	203	37.577	30.536	46.763	1.00	5.13	6
ATOM	1669	OH	TYR	A	203	37.355	31.607	45.918	1.00	5.71	8
ATOM	1670	C	TYR	A	203	38.899	26.963	51.897	1.00	5.73	6
ATOM	1671	O	TYR	A	203	37.783	26.505	52.205	1.00	5.91	8
ATOM	1672	N	ASP	A	204	39.942	26.807	52.703	1.00	6.06	7
ATOM	1673	CA	ASP	A	204	39.883	26.202	54.010	1.00	6.93	6
ATOM	1674	CB	ASP	A	204	41.108	25.454	54.543	1.00	7.71	6
ATOM	1675	CG	ASP	A	204	41.389	24.192	53.738	1.00	9.87	6
ATOM	1676	OD1	ASP	A	204	40.413	23.443	53.469	1.00	11.60	8
ATOM	1677	OD2	ASP	A	204	42.553	23.870	53.354	1.00	10.31	8
ATOM	1678	C	ASP	A	204	39.632	27.395	55.016	1.00	7.25	6
ATOM	1679	O	ASP	A	204	39.231	27.113	56.154	1.00	7.19	8
ATOM	1680	N	HIS	A	205	39.838	28.671	54.654	1.00	7.01	7
ATOM	1681	CA	HIS	A	205	39.660	29.773	55.659	1.00	7.00	6
ATOM	1682	CB	HIS	A	205	40.519	30.961	55.174	1.00	5.97	6
ATOM	1683	CG	HIS	A	205	40.566	32.025	56.220	1.00	7.15	6
ATOM	1684	CD2	HIS	A	205	39.590	32.773	56.780	1.00	5.16	6
ATOM	1685	ND1	HIS	A	205	41.751	32.331	56.910	1.00	8.31	7
ATOM	1686	CE1	HIS	A	205	41.525	33.260	57.828	1.00	6.29	6
ATOM	1687	NE2	HIS	A	205	40.214	33.513	57.752	1.00	8.24	7
ATOM	1688	C	HIS	A	205	38.199	30.050	55.824	1.00	7.15	6
ATOM	1689	O	HIS	A	205	37.511	30.307	54.825	1.00	7.72	8
ATOM	1690	N	PRO	A	206	37.579	29.986	56.988	1.00	6.98	7
ATOM	1691	CD	PRO	A	206	38.242	29.637	58.262	1.00	6.83	6
ATOM	1692	CA	PRO	A	206	36.134	30.164	57.160	1.00	6.77	6
ATOM	1693	CB	PRO	A	206	35.776	29.837	58.641	1.00	6.82	6
ATOM	1694	CG	PRO	A	206	37.146	30.071	59.263	1.00	6.98	6
ATOM	1695	C	PRO	A	206	35.653	31.549	56.764	1.00	6.49	6
ATOM	1696	O	PRO	A	206	34.527	31.608	56.238	1.00	6.33	8

ATOM	1697	N	ASP	A	207	36.466	32.591	56.971	1.00	6.12	7
ATOM	1698	CA	ASP	A	207	36.056	33.949	56.613	1.00	6.05	6
ATOM	1699	CB	ASP	A	207	36.954	35.059	57.168	1.00	6.37	6
ATOM	1700	CG	ASP	A	207	36.964	35.075	58.705	1.00	6.87	6
ATOM	1701	OD1	ASP	A	207	36.208	34.392	59.396	1.00	6.00	8
ATOM	1702	OD2	ASP	A	207	37.779	35.836	59.261	1.00	7.95	8
ATOM	1703	C	ASP	A	207	36.033	34.139	55.096	1.00	6.17	6
ATOM	1704	O	ASP	A	207	35.225	34.906	54.573	1.00	5.78	8
ATOM	1705	N	VAL	A	208	36.985	33.441	54.427	1.00	6.47	7
ATOM	1706	CA	VAL	A	208	37.054	33.472	52.973	1.00	6.58	6
ATOM	1707	CB	VAL	A	208	38.353	32.859	52.465	1.00	7.47	6
ATOM	1708	CG1	VAL	A	208	38.292	32.594	50.949	1.00	7.06	6
ATOM	1709	CG2	VAL	A	208	39.526	33.788	52.805	1.00	6.71	6
ATOM	1710	C	VAL	A	208	35.795	32.784	52.426	1.00	6.90	6
ATOM	1711	O	VAL	A	208	35.103	33.349	51.530	1.00	6.95	8
ATOM	1712	N	VAL	A	209	35.436	31.598	52.923	1.00	6.93	7
ATOM	1713	CA	VAL	A	209	34.257	30.881	52.457	1.00	7.00	6
ATOM	1714	CB	VAL	A	209	34.140	29.527	53.170	1.00	5.34	6
ATOM	1715	CG1	VAL	A	209	32.865	28.784	52.814	1.00	5.00	6
ATOM	1716	CG2	VAL	A	209	35.346	28.638	52.878	1.00	5.00	6
ATOM	1717	C	VAL	A	209	32.996	31.743	52.652	1.00	7.32	6
ATOM	1718	O	VAL	A	209	32.199	31.882	51.684	1.00	7.35	8
ATOM	1719	N	ALA	A	210	32.798	32.341	53.838	1.00	7.34	7
ATOM	1720	CA	ALA	A	210	31.623	33.165	54.102	1.00	7.52	6
ATOM	1721	CB	ALA	A	210	31.558	33.591	55.584	1.00	7.62	6
ATOM	1722	C	ALA	A	210	31.490	34.416	53.261	1.00	7.58	6
ATOM	1723	O	ALA	A	210	30.401	34.806	52.803	1.00	7.48	8
ATOM	1724	N	GLU	A	211	32.614	35.095	53.060	1.00	7.67	7
ATOM	1725	CA	GLU	A	211	32.662	36.296	52.216	1.00	7.90	6
ATOM	1726	CB	GLU	A	211	34.061	36.946	52.363	1.00	9.96	6
ATOM	1727	CG	GLU	A	211	34.267	38.168	51.517	1.00	13.89	6
ATOM	1728	CD	GLU	A	211	33.197	39.270	51.640	1.00	16.28	6
ATOM	1729	OE1	GLU	A	211	32.845	39.772	50.515	1.00	18.47	8
ATOM	1730	OE2	GLU	A	211	32.747	39.610	52.771	1.00	13.34	8
ATOM	1731	C	GLU	A	211	32.384	36.053	50.721	1.00	7.61	6
ATOM	1732	O	GLU	A	211	31.758	36.890	50.060	1.00	7.56	8
ATOM	1733	N	THR	A	212	32.907	34.960	50.184	1.00	7.17	7
ATOM	1734	CA	THR	A	212	32.727	34.572	48.781	1.00	6.96	6
ATOM	1735	CB	THR	A	212	33.705	33.464	48.413	1.00	8.17	6
ATOM	1736	OG1	THR	A	212	35.056	33.934	48.636	1.00	9.40	8
ATOM	1737	CG2	THR	A	212	33.660	33.139	46.939	1.00	7.69	6
ATOM	1738	C	THR	A	212	31.276	34.155	48.564	1.00	6.87	6
ATOM	1739	O	THR	A	212	30.724	34.456	47.522	1.00	6.69	8
ATOM	1740	N	LYS	A	213	30.604	33.516	49.527	1.00	6.92	7
ATOM	1741	CA	LYS	A	213	29.168	33.214	49.424	1.00	7.14	6
ATOM	1742	CB	LYS	A	213	28.634	32.331	50.553	1.00	6.97	6
ATOM	1743	CG	LYS	A	213	29.076	30.863	50.321	1.00	9.06	6
ATOM	1744	CD	LYS	A	213	28.605	30.065	51.592	1.00	9.86	6
ATOM	1745	CE	LYS	A	213	29.312	28.701	51.442	1.00	10.33	6
ATOM	1746	NZ	LYS	A	213	28.914	27.848	52.609	1.00	11.44	7
ATOM	1747	C	LYS	A	213	28.352	34.524	49.417	1.00	7.15	6
ATOM	1748	O	LYS	A	213	27.462	34.755	48.620	1.00	6.94	8
ATOM	1749	N	LYS	A	214	28.687	35.476	50.279	1.00	7.01	7
ATOM	1750	CA	LYS	A	214	28.061	36.774	50.337	1.00	7.39	6
ATOM	1751	CB	LYS	A	214	28.638	37.530	51.539	1.00	11.90	6
ATOM	1752	CG	LYS	A	214	28.423	39.011	51.741	1.00	17.64	6
ATOM	1753	CD	LYS	A	214	29.354	39.548	52.915	1.00	22.01	6
ATOM	1754	CE	LYS	A	214	29.770	41.017	52.697	1.00	24.62	6
ATOM	1755	NZ	LYS	A	214	31.138	41.472	53.171	1.00	24.85	7
ATOM	1756	C	LYS	A	214	28.290	37.533	49.021	1.00	7.07	6
ATOM	1757	O	LYS	A	214	27.317	38.174	48.561	1.00	7.02	8
ATOM	1758	N	TRP	A	215	29.481	37.502	48.430	1.00	6.68	7
ATOM	1759	CA	TRP	A	215	29.726	38.173	47.140	1.00	6.58	6
ATOM	1760	CB	TRP	A	215	31.216	38.139	46.715	1.00	5.00	6
ATOM	1761	CG	TRP	A	215	31.353	38.622	45.281	1.00	5.00	6
ATOM	1762	CD2	TRP	A	215	31.418	37.741	44.122	1.00	5.00	6
ATOM	1763	CE2	TRP	A	215	31.427	38.544	43.003	1.00	5.00	6
ATOM	1764	CE3	TRP	A	215	31.455	36.349	43.980	1.00	5.00	6
ATOM	1765	CD1	TRP	A	215	31.355	39.909	44.808	1.00	5.00	6
ATOM	1766	NE1	TRP	A	215	31.418	39.874	43.430	1.00	5.00	7
ATOM	1767	CZ2	TRP	A	215	31.507	38.008	41.720	1.00	5.00	6
ATOM	1768	CZ3	TRP	A	215	31.494	35.789	42.707	1.00	5.18	6
ATOM	1769	CH2	TRP	A	215	31.534	36.649	41.559	1.00	5.00	6
ATOM	1770	C	TRP	A	215	28.836	37.573	46.045	1.00	6.80	6
ATOM	1771	O	TRP	A	215	28.222	38.231	45.223	1.00	6.73	8
ATOM	1772	N	GLY	A	216	28.714	36.209	46.000	1.00	7.00	7
ATOM	1773	CA	GLY	A	216	27.936	35.541	45.004	1.00	7.12	6
ATOM	1774	C	GLY	A	216	26.482	35.990	44.999	1.00	7.24	6
ATOM	1775	O	GLY	A	216	25.868	36.132	43.918	1.00	6.99	8
ATOM	1776	N	ILE	A	217	25.955	36.136	46.205	1.00	7.41	7
ATOM	1777	CA	ILE	A	217	24.531	36.546	46.325	1.00	7.50	6
ATOM	1778	CB	ILE	A	217	24.011	36.340	47.777	1.00	8.38	6
ATOM	1779	CG2	ILE	A	217	22.627	36.981	48.057	1.00	6.66	6
ATOM	1780	CG1	ILE	A	217	23.923	34.851	48.131	1.00	7.56	6
ATOM	1781	CD1	ILE	A	217	24.065	34.682	49.629	1.00	7.44	6
ATOM	1782	C	ILE	A	217	24.406	37.971	45.846	1.00	7.47	6
ATOM	1783	O	ILE	A	217	23.541	38.350	45.092	1.00	7.49	8
ATOM	1784	N	TRP	A	218	25.329	38.844	46.222	1.00	7.72	7
ATOM	1785	CA	TRP	A	218	25.354	40.252	45.814	1.00	7.84	6
ATOM	1786	CB	TRP	A	218	26.556	40.953	46.464	1.00	7.78	6
ATOM	1787	CG	TRP	A	218	26.778	42.365	45.975	1.00	8.77	6
ATOM	1788	CD2	TRP	A	218	27.638	42.809	44.926	1.00	8.24	6
ATOM	1789	CE2	TRP	A	218	27.466	44.221	44.817	1.00	9.24	6
ATOM	1790	CE3	TRP	A	218	28.514	42.168	44.041	1.00	7.35	6
ATOM	1791	CD1	TRP	A	218	26.112	43.473	46.439	1.00	9.49	6
ATOM	1792	NE1	TRP	A	218	26.535	44.589	45.737	1.00	9.30	7
ATOM	1793	CZ2	TRP	A	218	28.169	45.022	43.903	1.00	8.69	6
ATOM	1794	CZ3	TRP	A	218	29.215	42.962	43.149	1.00	7.92	6
ATOM	1795	CH2	TRP	A	218	29.058	44.371	43.069	1.00	8.47	6
ATOM	1796	C	TRP	A	218	25.395	40.438	44.301	1.00	7.81	6
ATOM	1797	O	TRP	A	218	24.708	41.250	43.686	1.00	7.56	8
ATOM	1798	N	TYR	A	219	26.300	39.722	43.653	1.00	8.18	7
ATOM	1799	CA	TYR	A	219	26.537	39.709	42.203	1.00	8.37	6
ATOM	1800	CB	TYR	A	219	27.703	38.789	41.955	1.00	8.61	6
ATOM	1801	CG	TYR	A	219	28.243	38.670	40.554	1.00	9.11	6
ATOM	1802	CD1	TYR	A	219	28.615	39.784	39.810	1.00	9.59	6

ATOM	1803	CE1	TYR	A	219	29.180	39.619	38.541	1.00	9.96	6
ATOM	1804	CD2	TYR	A	219	28.416	37.404	40.008	1.00	9.35	6
ATOM	1805	CE2	TYR	A	219	28.959	37.265	38.740	1.00	9.78	6
ATOM	1806	CZ	TYR	A	219	29.346	38.361	38.021	1.00	10.19	6
ATOM	1807	OH	TYR	A	219	29.899	38.187	36.757	1.00	11.08	8
ATOM	1808	C	TYR	A	219	25.279	39.259	41.447	1.00	8.69	6
ATOM	1809	O	TYR	A	219	24.836	39.946	40.527	1.00	8.37	8
ATOM	1810	N	ALA	A	220	24.676	38.131	41.869	1.00	9.13	7
ATOM	1811	CA	ALA	A	220	23.427	37.644	41.267	1.00	9.77	6
ATOM	1812	CB	ALA	A	220	22.899	36.384	41.981	1.00	8.61	6
ATOM	1813	C	ALA	A	220	22.315	38.685	41.321	1.00	10.07	6
ATOM	1814	O	ALA	A	220	21.536	38.887	40.377	1.00	10.05	8
ATOM	1815	N	ASN	A	221	22.192	39.338	42.473	1.00	10.39	7
ATOM	1816	CA	ASN	A	221	21.200	40.374	42.757	1.00	10.66	6
ATOM	1817	CB	ASN	A	221	21.013	40.698	44.262	1.00	13.90	6
ATOM	1818	CG	ASN	A	221	20.192	39.543	44.855	1.00	18.18	6
ATOM	1819	OD1	ASN	A	221	19.371	38.852	44.227	1.00	19.46	8
ATOM	1820	ND2	ASN	A	221	20.481	39.263	46.125	1.00	19.86	7
ATOM	1821	C	ASN	A	221	21.524	41.717	42.136	1.00	10.51	6
ATOM	1822	O	ASN	A	221	20.592	42.323	41.626	1.00	10.40	8
ATOM	1823	N	GLU	A	222	22.794	42.125	42.143	1.00	10.51	7
ATOM	1824	CA	GLU	A	222	23.160	43.432	41.552	1.00	10.18	6
ATOM	1825	CB	GLU	A	222	24.621	43.807	41.791	1.00	11.08	6
ATOM	1826	CG	GLU	A	222	25.013	45.244	41.469	1.00	12.96	6
ATOM	1827	CD	GLU	A	222	24.412	46.203	42.496	1.00	15.13	6
ATOM	1828	OE1	GLU	A	222	23.947	45.777	43.576	1.00	15.79	8
ATOM	1829	OE2	GLU	A	222	24.381	47.432	42.254	1.00	16.17	8
ATOM	1830	C	GLU	A	222	22.903	43.428	40.052	1.00	9.82	6
ATOM	1831	O	GLU	A	222	22.470	44.444	39.507	1.00	9.72	8
ATOM	1832	N	LEU	A	223	23.227	42.343	39.348	1.00	9.48	7
ATOM	1833	CA	LEU	A	223	23.009	42.319	37.909	1.00	9.43	6
ATOM	1834	CB	LEU	A	223	24.300	41.715	37.281	1.00	7.13	6
ATOM	1835	CG	LEU	A	223	25.595	42.503	37.476	1.00	5.72	6
ATOM	1836	CD1	LEU	A	223	26.752	41.715	36.835	1.00	5.00	6
ATOM	1837	CD2	LEU	A	223	25.470	43.888	36.880	1.00	5.20	6
ATOM	1838	C	LEU	A	223	21.794	41.550	37.456	1.00	9.44	6
ATOM	1839	O	LEU	A	223	21.561	41.335	36.280	1.00	9.57	8
ATOM	1840	N	SER	A	224	20.953	40.998	38.286	1.00	9.74	7
ATOM	1841	CA	SER	A	224	19.825	40.156	37.925	1.00	10.06	6
ATOM	1842	CB	SER	A	224	18.660	40.832	37.156	1.00	14.91	6
ATOM	1843	OG	SER	A	224	18.251	41.991	37.901	1.00	19.93	8
ATOM	1844	C	SER	A	224	20.293	38.979	37.047	1.00	9.76	6
ATOM	1845	O	SER	A	224	19.648	38.752	36.004	1.00	9.74	8
ATOM	1846	N	LEU	A	225	21.340	38.248	37.445	1.00	9.20	7
ATOM	1847	CA	LEU	A	225	21.770	37.113	36.651	1.00	8.94	6
ATOM	1848	CB	LEU	A	225	23.164	36.688	37.088	1.00	10.36	6
ATOM	1849	CG	LEU	A	225	24.297	37.738	36.958	1.00	11.62	6
ATOM	1850	CD1	LEU	A	225	25.552	37.149	37.597	1.00	10.68	6
ATOM	1851	CD2	LEU	A	225	24.524	38.163	35.508	1.00	10.53	6
ATOM	1852	C	LEU	A	225	20.793	35.945	36.827	1.00	8.77	6
ATOM	1853	O	LEU	A	225	20.084	35.785	37.796	1.00	8.44	8
ATOM	1854	N	ASP	A	226	20.734	35.084	35.804	1.00	8.55	7
ATOM	1855	CA	ASP	A	226	19.950	33.911	35.674	1.00	7.98	6
ATOM	1856	CB	ASP	A	226	19.357	33.821	34.254	1.00	7.73	6
ATOM	1857	CG	ASP	A	226	18.559	35.071	33.990	1.00	7.95	6
ATOM	1858	OD1	ASP	A	226	17.512	35.272	34.681	1.00	10.67	8
ATOM	1859	OD2	ASP	A	226	18.962	35.869	33.172	1.00	7.61	8
ATOM	1860	C	ASP	A	226	20.796	32.668	35.806	1.00	7.95	6
ATOM	1861	O	ASP	A	226	20.213	31.578	35.837	1.00	8.41	8
ATOM	1862	N	GLY	A	227	22.107	32.836	35.852	1.00	7.65	7
ATOM	1863	CA	GLY	A	227	22.992	31.679	35.946	1.00	7.46	6
ATOM	1864	C	GLY	A	227	24.471	32.049	35.990	1.00	7.30	6
ATOM	1865	O	GLY	A	227	24.880	33.197	36.042	1.00	6.95	8
ATOM	1866	N	PHE	A	228	25.294	30.990	36.029	1.00	7.33	7
ATOM	1867	CA	PHE	A	228	26.742	31.170	36.146	1.00	7.35	6
ATOM	1868	CB	PHE	A	228	27.220	30.898	37.558	1.00	6.74	6
ATOM	1869	CG	PHE	A	228	26.640	31.708	38.672	1.00	9.48	6
ATOM	1870	CD1	PHE	A	228	25.930	31.082	39.700	1.00	9.82	6
ATOM	1871	CD2	PHE	A	228	26.800	33.097	38.702	1.00	8.78	6
ATOM	1872	CE1	PHE	A	228	25.415	31.869	40.731	1.00	10.75	6
ATOM	1873	CE2	PHE	A	228	26.277	33.860	39.746	1.00	9.42	6
ATOM	1874	CZ	PHE	A	228	25.590	33.241	40.786	1.00	9.64	6
ATOM	1875	C	PHE	A	228	27.603	30.229	35.304	1.00	7.29	6
ATOM	1876	O	PHE	A	228	27.245	29.086	34.995	1.00	7.76	8
ATOM	1877	N	ARG	A	229	28.791	30.675	34.978	1.00	6.86	7
ATOM	1878	CA	ARG	A	229	29.818	29.927	34.305	1.00	6.75	6
ATOM	1879	CB	ARG	A	229	30.172	30.439	32.885	1.00	6.68	6
ATOM	1880	CG	ARG	A	229	31.309	29.551	32.327	1.00	5.59	6
ATOM	1881	CD	ARG	A	229	32.646	30.283	32.584	1.00	7.41	6
ATOM	1882	NE	ARG	A	229	33.701	29.623	31.828	1.00	7.61	7
ATOM	1883	CZ	ARG	A	229	34.985	29.905	31.872	1.00	8.29	6
ATOM	1884	NH1	ARG	A	229	35.833	29.189	31.139	1.00	7.90	7
ATOM	1885	NH2	ARG	A	229	35.388	30.913	32.626	1.00	7.66	7
ATOM	1886	C	ARG	A	229	30.998	29.916	35.323	1.00	6.49	6
ATOM	1887	O	ARG	A	229	31.518	30.980	35.697	1.00	6.39	8
ATOM	1888	N	ILE	A	230	31.427	28.711	35.760	1.00	6.19	7
ATOM	1889	CA	ILE	A	230	32.530	28.667	36.752	1.00	5.82	6
ATOM	1890	CB	ILE	A	230	32.239	27.598	37.860	1.00	6.87	6
ATOM	1891	CG2	ILE	A	230	33.534	27.325	38.636	1.00	5.00	6
ATOM	1892	CG1	ILE	A	230	31.001	28.126	38.637	1.00	6.60	6
ATOM	1893	CD1	ILE	A	230	30.470	27.073	39.606	1.00	11.75	6
ATOM	1894	C	ILE	A	230	33.907	28.409	36.148	1.00	5.56	6
ATOM	1895	O	ILE	A	230	34.225	27.368	35.555	1.00	5.42	8
ATOM	1896	N	ASP	A	231	34.758	29.428	36.246	1.00	5.02	7
ATOM	1897	CA	ASP	A	231	36.086	29.322	35.714	1.00	5.00	6
ATOM	1898	CB	ASP	A	231	36.693	30.746	35.684	1.00	5.00	6
ATOM	1899	CG	ASP	A	231	38.078	30.857	35.062	1.00	5.00	6
ATOM	1900	OD1	ASP	A	231	38.156	30.584	33.864	1.00	5.00	8
ATOM	1901	OD2	ASP	A	231	39.013	31.237	35.828	1.00	5.00	8
ATOM	1902	C	ASP	A	231	37.016	28.427	36.518	1.00	5.00	6
ATOM	1903	O	ASP	A	231	36.987	28.462	37.750	1.00	5.00	8
ATOM	1904	N	ALA	A	232	37.861	27.681	35.819	1.00	5.00	7
ATOM	1905	CA	ALA	A	232	38.889	26.846	36.430	1.00	5.00	6
ATOM	1906	CB	ALA	A	232	39.930	27.869	36.945	1.00	6.65	6
ATOM	1907	C	ALA	A	232	38.515	25.954	37.593	1.00	5.00	6
ATOM	1908	O	ALA	A	232	39.189	25.916	38.626	1.00	5.00	8

ATOM	1909	N	ALA	A	233	37.399	25.223	37.414	1.00	5.00	7
ATOM	1910	CA	ALA	A	233	36.848	24.420	38.465	1.00	5.45	6
ATOM	1911	CB	ALA	A	233	35.529	23.866	37.899	1.00	6.05	6
ATOM	1912	C	ALA	A	233	37.755	23.310	38.952	1.00	6.00	6
ATOM	1913	O	ALA	A	233	37.565	22.963	40.144	1.00	6.16	8
ATOM	1914	N	LYS	A	234	38.683	22.764	38.169	1.00	5.81	7
ATOM	1915	CA	LYS	A	234	39.508	21.670	38.618	1.00	6.08	6
ATOM	1916	CB	LYS	A	234	40.171	20.929	37.485	1.00	5.76	6
ATOM	1917	CG	LYS	A	234	41.275	21.620	36.704	1.00	6.41	6
ATOM	1918	CD	LYS	A	234	41.843	20.613	35.671	1.00	7.10	6
ATOM	1919	CE	LYS	A	234	43.118	21.208	34.994	1.00	5.42	6
ATOM	1920	NZ	LYS	A	234	43.541	20.287	33.901	1.00	5.00	7
ATOM	1921	C	LYS	A	234	40.530	22.145	39.648	1.00	6.60	6
ATOM	1922	O	LYS	A	234	41.110	21.289	40.336	1.00	6.53	8
ATOM	1923	N	HIS	A	235	40.709	23.486	39.781	1.00	6.73	7
ATOM	1924	CA	HIS	A	235	41.640	23.999	40.796	1.00	6.75	6
ATOM	1925	CB	HIS	A	235	42.497	25.195	40.296	1.00	6.58	6
ATOM	1926	CG	HIS	A	235	43.030	24.789	38.959	1.00	6.14	6
ATOM	1927	CD2	HIS	A	235	42.575	25.085	37.724	1.00	7.29	6
ATOM	1928	ND1	HIS	A	235	44.084	23.935	38.789	1.00	5.80	7
ATOM	1929	CE1	HIS	A	235	44.290	23.756	37.502	1.00	7.11	6
ATOM	1930	NE2	HIS	A	235	43.386	24.446	36.829	1.00	6.22	7
ATOM	1931	C	HIS	A	235	40.857	24.459	42.002	1.00	6.76	6
ATOM	1932	O	HIS	A	235	41.512	25.042	42.814	1.00	6.54	8
ATOM	1933	N	ILE	A	236	39.583	24.341	42.255	1.00	6.68	7
ATOM	1934	CA	ILE	A	236	38.916	24.866	43.434	1.00	6.87	6
ATOM	1935	CB	ILE	A	236	37.858	25.949	43.026	1.00	5.00	6
ATOM	1936	CG2	ILE	A	236	37.089	26.450	44.213	1.00	5.00	6
ATOM	1937	CG1	ILE	A	236	38.558	27.103	42.238	1.00	5.00	6
ATOM	1938	CD1	ILE	A	236	37.601	27.999	41.485	1.00	5.00	6
ATOM	1939	C	ILE	A	236	38.228	23.724	44.193	1.00	7.20	6
ATOM	1940	O	ILE	A	236	37.587	22.852	43.555	1.00	7.08	8
ATOM	1941	N	LYS	A	237	38.407	23.693	45.498	1.00	7.57	7
ATOM	1942	CA	LYS	A	237	37.831	22.688	46.424	1.00	7.74	6
ATOM	1943	CB	LYS	A	237	37.828	23.257	47.868	1.00	9.45	6
ATOM	1944	CG	LYS	A	237	37.355	22.233	48.831	1.00	12.16	6
ATOM	1945	CD	LYS	A	237	37.037	22.463	50.263	1.00	15.99	6
ATOM	1946	CE	LYS	A	237	37.992	23.114	51.189	1.00	19.56	6
ATOM	1947	NZ	LYS	A	237	37.579	22.767	52.623	1.00	22.41	7
ATOM	1948	C	LYS	A	237	36.425	22.314	45.956	1.00	7.39	6
ATOM	1949	O	LYS	A	237	35.561	23.187	45.849	1.00	6.92	8
ATOM	1950	N	PHE	A	238	36.210	21.062	45.551	1.00	7.45	7
ATOM	1951	CA	PHE	A	238	34.912	20.689	44.944	1.00	7.67	6
ATOM	1952	CB	PHE	A	238	34.921	19.232	44.425	1.00	8.77	6
ATOM	1953	CG	PHE	A	238	35.992	18.884	43.442	1.00	9.75	6
ATOM	1954	CD1	PHE	A	238	36.688	19.851	42.716	1.00	9.45	6
ATOM	1955	CD2	PHE	A	238	36.262	17.529	43.199	1.00	10.39	6
ATOM	1956	CE1	PHE	A	238	37.638	19.448	41.787	1.00	9.12	6
ATOM	1957	CE2	PHE	A	238	37.220	17.125	42.292	1.00	8.83	6
ATOM	1958	CZ	PHE	A	238	37.882	18.097	41.562	1.00	9.31	6
ATOM	1959	C	PHE	A	238	33.694	20.870	45.841	1.00	7.61	6
ATOM	1960	O	PHE	A	238	32.666	21.356	45.350	1.00	7.47	8
ATOM	1961	N	SER	A	239	33.801	20.475	47.113	1.00	7.50	7
ATOM	1962	CA	SER	A	239	32.706	20.656	48.065	1.00	7.57	6
ATOM	1963	CB	SER	A	239	32.940	19.984	49.417	1.00	7.79	6
ATOM	1964	OG	SER	A	239	34.169	20.443	49.919	1.00	10.61	8
ATOM	1965	C	SER	A	239	32.410	22.159	48.249	1.00	7.33	6
ATOM	1966	O	SER	A	239	31.237	22.448	48.454	1.00	7.20	8
ATOM	1967	N	PHE	A	240	33.380	23.066	48.168	1.00	7.19	7
ATOM	1968	CA	PHE	A	240	33.073	24.471	48.275	1.00	7.28	6
ATOM	1969	CB	PHE	A	240	34.332	25.325	48.382	1.00	7.42	6
ATOM	1970	CG	PHE	A	240	34.049	26.801	48.123	1.00	7.00	6
ATOM	1971	CD1	PHE	A	240	33.390	27.560	49.085	1.00	6.31	6
ATOM	1972	CD2	PHE	A	240	34.413	27.352	46.911	1.00	6.51	6
ATOM	1973	CE1	PHE	A	240	33.091	28.886	48.775	1.00	7.11	6
ATOM	1974	CE2	PHE	A	240	34.116	28.674	46.615	1.00	5.97	6
ATOM	1975	CZ	PHE	A	240	33.479	29.440	47.555	1.00	5.18	6
ATOM	1976	C	PHE	A	240	32.259	24.900	47.044	1.00	7.56	6
ATOM	1977	O	PHE	A	240	31.251	25.631	47.191	1.00	7.63	8
ATOM	1978	N	LEU	A	241	32.639	24.464	45.838	1.00	7.46	7
ATOM	1979	CA	LEU	A	241	31.880	24.877	44.661	1.00	7.91	6
ATOM	1980	CB	LEU	A	241	32.528	24.553	43.318	1.00	5.00	6
ATOM	1981	CG	LEU	A	241	33.814	25.279	42.944	1.00	5.00	6
ATOM	1982	CD1	LEU	A	241	34.520	24.613	41.753	1.00	5.00	6
ATOM	1983	CD2	LEU	A	241	33.548	26.754	42.654	1.00	5.00	6
ATOM	1984	C	LEU	A	241	30.418	24.377	44.720	1.00	8.46	6
ATOM	1985	O	LEU	A	241	29.483	25.127	44.303	1.00	8.58	8
ATOM	1986	N	ARG	A	242	30.184	23.164	45.219	1.00	8.61	7
ATOM	1987	CA	ARG	A	242	28.777	22.774	45.286	1.00	8.92	6
ATOM	1988	CB	ARG	A	242	28.716	21.286	45.431	1.00	10.58	6
ATOM	1989	CG	ARG	A	242	28.819	20.546	46.608	1.00	12.57	6
ATOM	1990	CD	ARG	A	242	27.687	19.642	47.094	1.00	13.52	6
ATOM	1991	NE	ARG	A	242	28.192	19.629	48.476	1.00	15.26	7
ATOM	1992	CZ	ARG	A	242	28.955	18.913	49.256	1.00	17.48	6
ATOM	1993	NH1	ARG	A	242	29.464	17.761	48.866	1.00	19.52	7
ATOM	1994	NH2	ARG	A	242	29.303	19.285	50.505	1.00	18.04	7
ATOM	1995	C	ARG	A	242	28.042	23.548	46.379	1.00	8.91	6
ATOM	1996	O	ARG	A	242	26.891	23.909	46.129	1.00	8.59	8
ATOM	1997	N	ASP	A	243	28.653	23.828	47.526	1.00	9.00	7
ATOM	1998	CA	ASP	A	243	27.964	24.591	48.533	1.00	9.47	6
ATOM	1999	CB	ASP	A	243	28.812	24.581	49.811	1.00	11.98	6
ATOM	2000	CG	ASP	A	243	28.766	23.183	50.417	1.00	15.20	6
ATOM	2001	OD1	ASP	A	243	29.580	22.982	51.372	1.00	19.21	8
ATOM	2002	OD2	ASP	A	243	28.049	22.251	50.036	1.00	13.33	8
ATOM	2003	C	ASP	A	243	27.798	26.049	48.117	1.00	9.53	6
ATOM	2004	O	ASP	A	243	26.797	26.664	48.539	1.00	9.54	8
ATOM	2005	N	TRP	A	244	28.755	26.581	47.303	1.00	9.34	7
ATOM	2006	CA	TRP	A	244	28.622	28.005	46.908	1.00	9.20	6
ATOM	2007	CB	TRP	A	244	29.862	28.511	46.195	1.00	7.34	6
ATOM	2008	CG	TRP	A	244	29.831	29.924	45.719	1.00	8.91	6
ATOM	2009	CD2	TRP	A	244	29.442	30.367	44.411	1.00	9.51	6
ATOM	2010	CE2	TRP	A	244	29.589	31.773	44.384	1.00	10.54	6
ATOM	2011	CE3	TRP	A	244	29.020	29.698	43.243	1.00	10.38	6
ATOM	2012	CD1	TRP	A	244	30.168	31.065	46.419	1.00	9.07	6
ATOM	2013	NE1	TRP	A	244	30.036	32.191	45.638	1.00	9.59	7
ATOM	2014	CZ2	TRP	A	244	29.289	32.524	43.219	1.00	9.81	6

ATOM	2015	CZ3	TRP	A	244	28.727	30.446	42.096	1.00	10.45	6
ATOM	2016	CH2	TRP	A	244	28.862	31.859	42.106	1.00	9.71	6
ATOM	2017	C	TRP	A	244	27.386	28.200	46.006	1.00	9.28	6
ATOM	2018	O	TRP	A	244	26.651	29.168	46.164	1.00	8.82	8
ATOM	2019	N	VAL	A	245	27.217	27.284	45.056	1.00	9.64	7
ATOM	2020	CA	VAL	A	245	26.082	27.305	44.114	1.00	10.52	6
ATOM	2021	CB	VAL	A	245	26.108	26.185	43.039	1.00	12.05	6
ATOM	2022	CG1	VAL	A	245	24.832	26.113	42.198	1.00	13.84	6
ATOM	2023	CG2	VAL	A	245	27.262	26.450	42.081	1.00	13.35	6
ATOM	2024	C	VAL	A	245	24.722	27.203	44.853	1.00	10.63	6
ATOM	2025	O	VAL	A	245	23.758	27.906	44.590	1.00	10.02	8
ATOM	2026	N	GLN	A	246	24.745	26.269	45.790	1.00	11.30	7
ATOM	2027	CA	GLN	A	246	23.552	26.022	46.634	1.00	12.37	6
ATOM	2028	CB	GLN	A	246	23.878	24.727	47.381	1.00	18.96	6
ATOM	2029	CG	GLN	A	246	22.737	24.176	48.214	1.00	27.47	6
ATOM	2030	CD	GLN	A	246	23.367	23.366	49.350	1.00	34.63	6
ATOM	2031	OE1	GLN	A	246	22.842	23.446	50.493	1.00	37.91	8
ATOM	2032	NE2	GLN	A	246	24.476	22.642	49.028	1.00	36.61	7
ATOM	2033	C	GLN	A	246	23.153	27.225	47.485	1.00	12.39	6
ATOM	2034	O	GLN	A	246	21.970	27.561	47.531	1.00	12.22	8
ATOM	2035	N	ALA	A	247	24.083	27.968	48.099	1.00	12.46	7
ATOM	2036	CA	ALA	A	247	23.852	29.144	48.893	1.00	12.61	6
ATOM	2037	CB	ALA	A	247	25.094	29.791	49.517	1.00	12.47	6
ATOM	2038	C	ALA	A	247	23.231	30.263	48.050	1.00	12.74	6
ATOM	2039	O	ALA	A	247	22.308	30.857	48.561	1.00	12.85	8
ATOM	2040	N	VAL	A	248	23.710	30.495	46.838	1.00	12.75	7
ATOM	2041	CA	VAL	A	248	23.159	31.471	45.933	1.00	12.69	6
ATOM	2042	CB	VAL	A	248	24.009	31.688	44.684	1.00	11.87	6
ATOM	2043	CG1	VAL	A	248	23.357	32.721	43.754	1.00	12.19	6
ATOM	2044	CG2	VAL	A	248	25.400	32.171	45.014	1.00	11.42	6
ATOM	2045	C	VAL	A	248	21.748	31.040	45.537	1.00	12.91	6
ATOM	2046	O	VAL	A	248	20.866	31.889	45.506	1.00	12.81	8
ATOM	2047	N	ARG	A	249	21.483	29.791	45.237	1.00	13.31	7
ATOM	2048	CA	ARG	A	249	20.124	29.352	44.897	1.00	13.92	6
ATOM	2049	CB	ARG	A	249	20.066	27.906	44.404	1.00	11.75	6
ATOM	2050	CG	ARG	A	249	20.681	27.726	43.033	1.00	12.59	6
ATOM	2051	CD	ARG	A	249	20.814	26.274	42.576	1.00	12.82	6
ATOM	2052	NE	ARG	A	249	21.411	26.198	41.224	1.00	13.02	7
ATOM	2053	CZ	ARG	A	249	22.045	25.141	40.739	1.00	13.82	6
ATOM	2054	NH1	ARG	A	249	22.150	24.041	41.476	1.00	11.68	7
ATOM	2055	NH2	ARG	A	249	22.589	25.166	39.515	1.00	15.22	7
ATOM	2056	C	ARG	A	249	19.215	29.503	46.125	1.00	14.55	6
ATOM	2057	O	ARG	A	249	18.082	30.005	45.970	1.00	14.34	8
ATOM	2058	N	GLN	A	250	19.685	29.106	47.329	1.00	15.16	7
ATOM	2059	CA	GLN	A	250	18.794	29.252	48.498	1.00	15.83	6
ATOM	2060	CB	GLN	A	250	19.437	28.816	49.790	1.00	21.15	6
ATOM	2061	CG	GLN	A	250	18.902	27.566	50.460	1.00	28.24	6
ATOM	2062	CD	GLN	A	250	20.067	26.619	50.807	1.00	32.12	6
ATOM	2063	OE1	GLN	A	250	21.116	27.047	51.333	1.00	34.30	8
ATOM	2064	NE2	GLN	A	250	19.907	25.331	50.478	1.00	32.80	7
ATOM	2065	C	GLN	A	250	18.362	30.699	48.707	1.00	15.86	6
ATOM	2066	O	GLN	A	250	17.196	31.022	48.871	1.00	15.83	8
ATOM	2067	N	ALA	A	251	19.316	31.621	48.689	1.00	15.85	7
ATOM	2068	CA	ALA	A	251	19.029	33.029	48.862	1.00	16.06	6
ATOM	2069	CB	ALA	A	251	20.374	33.774	48.984	1.00	16.48	6
ATOM	2070	C	ALA	A	251	18.276	33.749	47.765	1.00	16.26	6
ATOM	2071	O	ALA	A	251	17.596	34.738	48.088	1.00	16.47	8
ATOM	2072	N	THR	A	252	18.343	33.433	46.476	1.00	16.21	7
ATOM	2073	CA	THR	A	252	17.631	34.224	45.487	1.00	16.03	6
ATOM	2074	CB	THR	A	252	18.462	34.328	44.189	1.00	13.96	6
ATOM	2075	OG1	THR	A	252	18.697	32.968	43.824	1.00	11.77	8
ATOM	2076	CG2	THR	A	252	19.776	35.060	44.281	1.00	12.34	6
ATOM	2077	C	THR	A	252	16.292	33.577	45.170	1.00	16.40	6
ATOM	2078	O	THR	A	252	15.441	34.281	44.670	1.00	16.40	8
ATOM	2079	N	GLY	A	253	16.139	32.267	45.429	1.00	16.68	7
ATOM	2080	CA	GLY	A	253	14.955	31.502	45.148	1.00	16.75	6
ATOM	2081	C	GLY	A	253	14.963	31.170	43.660	1.00	17.06	6
ATOM	2082	O	GLY	A	253	13.985	30.602	43.167	1.00	17.16	8
ATOM	2083	N	LYS	A	254	16.018	31.475	42.888	1.00	17.07	7
ATOM	2084	CA	LYS	A	254	16.045	31.196	41.437	1.00	16.76	6
ATOM	2085	CB	LYS	A	254	16.734	32.377	40.748	1.00	18.37	6
ATOM	2086	CG	LYS	A	254	16.007	33.685	40.568	1.00	21.23	6
ATOM	2087	CD	LYS	A	254	16.884	34.884	40.536	1.00	23.96	6
ATOM	2088	CE	LYS	A	254	17.330	35.674	39.332	1.00	25.51	6
ATOM	2089	NZ	LYS	A	254	18.369	36.723	39.792	1.00	27.00	7
ATOM	2090	C	LYS	A	254	16.731	29.871	41.097	1.00	16.34	6
ATOM	2091	O	LYS	A	254	17.533	29.323	41.896	1.00	16.45	8
ATOM	2092	N	GLU	A	255	16.459	29.313	39.928	1.00	15.71	7
ATOM	2093	CA	GLU	A	255	17.084	28.072	39.466	1.00	15.30	6
ATOM	2094	CB	GLU	A	255	16.504	27.668	38.102	1.00	18.71	6
ATOM	2095	CG	GLU	A	255	16.954	26.337	37.542	1.00	24.80	6
ATOM	2096	CD	GLU	A	255	16.927	26.270	36.020	1.00	29.50	6
ATOM	2097	OE1	GLU	A	255	16.083	26.965	35.393	1.00	31.45	8
ATOM	2098	OE2	GLU	A	255	17.730	25.553	35.340	1.00	31.98	8
ATOM	2099	C	GLU	A	255	18.623	28.183	39.365	1.00	14.27	6
ATOM	2100	O	GLU	A	255	19.417	27.324	39.733	1.00	14.14	8
ATOM	2101	N	MET	A	256	19.098	29.303	38.859	1.00	13.25	7
ATOM	2102	CA	MET	A	256	20.476	29.628	38.676	1.00	12.49	6
ATOM	2103	CB	MET	A	256	21.171	29.970	39.998	1.00	12.38	6
ATOM	2104	CG	MET	A	256	20.740	31.237	40.705	1.00	13.41	6
ATOM	2105	SD	MET	A	256	20.539	32.774	39.751	1.00	13.00	16
ATOM	2106	CE	MET	A	256	22.245	33.221	39.432	1.00	12.60	6
ATOM	2107	C	MET	A	256	21.209	28.486	37.966	1.00	11.87	6
ATOM	2108	O	MET	A	256	22.065	27.824	38.595	1.00	11.99	8
ATOM	2109	N	PHE	A	257	20.904	28.261	36.696	1.00	10.99	7
ATOM	2110	CA	PHE	A	257	21.612	27.238	35.914	1.00	10.24	6
ATOM	2111	CB	PHE	A	257	21.254	27.347	34.397	1.00	9.31	6
ATOM	2112	CG	PHE	A	257	22.056	26.339	33.591	1.00	9.08	6
ATOM	2113	CD1	PHE	A	257	21.634	25.032	33.491	1.00	7.86	6
ATOM	2114	CD2	PHE	A	257	23.248	26.741	32.991	1.00	8.44	6
ATOM	2115	CE1	PHE	A	257	22.425	24.132	32.769	1.00	9.31	6
ATOM	2116	CE2	PHE	A	257	24.059	25.861	32.292	1.00	9.08	6
ATOM	2117	CZ	PHE	A	257	23.624	24.537	32.171	1.00	10.03	6
ATOM	2118	C	PHE	A	257	23.115	27.439	36.047	1.00	9.70	6
ATOM	2119	O	PHE	A	257	23.583	28.593	35.876	1.00	9.75	8
ATOM	2120	N	THR	A	258	23.933	26.447	36.329	1.00	9.20	7

ATOM	2121	CA	THR	A	258	25.392	26.609	36.450	1.00	8.71	6
ATOM	2122	CB	THR	A	258	25.824	26.583	37.938	1.00	8.83	6
ATOM	2123	OG1	THR	A	258	25.203	27.678	38.617	1.00	7.38	8
ATOM	2124	CG2	THR	A	258	27.337	26.720	38.142	1.00	8.42	6
ATOM	2125	C	THR	A	258	26.136	25.533	35.646	1.00	8.29	6
ATOM	2126	O	THR	A	258	25.764	24.341	35.606	1.00	8.22	8
ATOM	2127	N	VAL	A	259	27.160	25.972	34.922	1.00	7.82	7
ATOM	2128	CA	VAL	A	259	28.001	25.077	34.102	1.00	7.47	6
ATOM	2129	CB	VAL	A	259	27.859	25.175	32.564	1.00	5.00	6
ATOM	2130	CG1	VAL	A	259	28.101	26.589	32.036	1.00	5.00	6
ATOM	2131	CG2	VAL	A	259	28.799	24.202	31.809	1.00	5.00	6
ATOM	2132	C	VAL	A	259	29.428	25.381	34.552	1.00	7.58	6
ATOM	2133	O	VAL	A	259	29.821	26.552	34.634	1.00	7.78	8
ATOM	2134	N	ALA	A	260	30.181	24.348	34.913	1.00	7.84	7
ATOM	2135	CA	ALA	A	260	31.555	24.487	35.346	1.00	8.08	6
ATOM	2136	CB	ALA	A	260	31.962	23.621	36.534	1.00	7.64	6
ATOM	2137	C	ALA	A	260	32.523	24.076	34.215	1.00	8.28	6
ATOM	2138	O	ALA	A	260	32.266	23.091	33.536	1.00	8.26	8
ATOM	2139	N	GLU	A	261	33.579	24.848	34.057	1.00	8.40	7
ATOM	2140	CA	GLU	A	261	34.628	24.574	33.125	1.00	8.60	6
ATOM	2141	CB	GLU	A	261	35.346	25.828	32.600	1.00	11.43	6
ATOM	2142	CG	GLU	A	261	36.281	25.350	31.518	1.00	17.13	6
ATOM	2143	CD	GLU	A	261	36.823	26.339	30.525	1.00	23.18	6
ATOM	2144	OE1	GLU	A	261	36.068	26.970	29.694	1.00	25.81	8
ATOM	2145	OE2	GLU	A	261	38.080	26.441	30.593	1.00	25.35	8
ATOM	2146	C	GLU	A	261	35.644	23.659	33.847	1.00	8.48	6
ATOM	2147	O	GLU	A	261	36.514	24.148	34.558	1.00	8.19	8
ATOM	2148	N	TYR	A	262	35.578	22.360	33.730	1.00	8.54	7
ATOM	2149	CA	TYR	A	262	36.500	21.387	34.293	1.00	8.87	6
ATOM	2150	CB	TYR	A	262	35.838	20.183	34.966	1.00	8.94	6
ATOM	2151	CG	TYR	A	262	36.761	19.321	35.821	1.00	9.11	6
ATOM	2152	CD1	TYR	A	262	36.660	19.322	37.206	1.00	9.01	6
ATOM	2153	CE1	TYR	A	262	37.509	18.576	37.984	1.00	9.15	6
ATOM	2154	CD2	TYR	A	262	37.743	18.497	35.253	1.00	9.44	6
ATOM	2155	CE2	TYR	A	262	38.605	17.723	36.026	1.00	9.65	6
ATOM	2156	CZ	TYR	A	262	38.490	17.788	37.415	1.00	9.42	6
ATOM	2157	OH	TYR	A	262	39.305	17.012	38.214	1.00	9.41	8
ATOM	2158	C	TYR	A	262	37.424	20.977	33.104	1.00	8.97	6
ATOM	2159	O	TYR	A	262	37.008	20.107	32.297	1.00	9.09	8
ATOM	2160	N	TRP	A	263	38.590	21.592	32.945	1.00	9.15	7
ATOM	2161	CA	TRP	A	263	39.403	21.292	31.774	1.00	9.76	6
ATOM	2162	CB	TRP	A	263	40.183	22.560	31.346	1.00	9.45	6
ATOM	2163	CG	TRP	A	263	40.638	22.366	29.917	1.00	11.66	6
ATOM	2164	CD2	TRP	A	263	39.892	22.703	28.733	1.00	12.75	6
ATOM	2165	CE2	TRP	A	263	40.662	22.299	27.612	1.00	13.78	6
ATOM	2166	CE3	TRP	A	263	38.631	23.289	28.512	1.00	12.04	6
ATOM	2167	CD1	TRP	A	263	41.800	21.810	29.466	1.00	12.57	6
ATOM	2168	NE1	TRP	A	263	41.820	21.731	28.078	1.00	13.80	7
ATOM	2169	CZ2	TRP	A	263	40.205	22.513	26.299	1.00	14.12	6
ATOM	2170	CZ3	TRP	A	263	38.201	23.453	27.210	1.00	10.77	6
ATOM	2171	CH2	TRP	A	263	38.970	23.094	26.122	1.00	11.88	6
ATOM	2172	C	TRP	A	263	40.303	20.053	31.833	1.00	10.24	6
ATOM	2173	O	TRP	A	263	41.436	20.018	32.294	1.00	10.30	8
ATOM	2174	N	GLN	A	264	39.758	18.950	31.301	1.00	10.57	7
ATOM	2175	CA	GLN	A	264	40.441	17.687	31.185	1.00	10.92	6
ATOM	2176	CB	GLN	A	264	40.619	16.999	32.536	1.00	14.66	6
ATOM	2177	CG	GLN	A	264	41.796	16.043	32.600	1.00	18.65	6
ATOM	2178	CD	GLN	A	264	41.972	15.344	33.934	1.00	22.60	6
ATOM	2179	OE1	GLN	A	264	41.214	15.481	34.907	1.00	24.23	8
ATOM	2180	NE2	GLN	A	264	42.996	14.478	34.047	1.00	23.90	7
ATOM	2181	C	GLN	A	264	39.681	16.811	30.191	1.00	11.04	6
ATOM	2182	O	GLN	A	264	38.461	16.643	30.232	1.00	10.83	8
ATOM	2183	N	ASN	A	265	40.454	16.216	29.289	1.00	11.25	7
ATOM	2184	CA	ASN	A	265	40.151	15.322	28.209	1.00	11.87	6
ATOM	2185	CB	ASN	A	265	41.223	15.365	27.078	1.00	11.52	6
ATOM	2186	CG	ASN	A	265	40.655	14.637	25.854	1.00	12.03	6
ATOM	2187	OD1	ASN	A	265	39.485	14.278	25.764	1.00	11.79	8
ATOM	2188	ND2	ASN	A	265	41.445	14.294	24.857	1.00	11.74	7
ATOM	2189	C	ASN	A	265	40.028	13.873	28.691	1.00	12.36	6
ATOM	2190	O	ASN	A	265	40.755	13.007	28.282	1.00	12.25	8
ATOM	2191	N	ASN	A	266	39.116	13.676	29.634	1.00	13.06	7
ATOM	2192	CA	ASN	A	266	38.844	12.428	30.337	1.00	13.75	6
ATOM	2193	CB	ASN	A	266	39.910	12.362	31.416	1.00	18.58	6
ATOM	2194	CG	ASN	A	266	40.150	11.016	32.031	1.00	22.56	6
ATOM	2195	OD1	ASN	A	266	41.311	10.519	31.969	1.00	26.43	8
ATOM	2196	ND2	ASN	A	266	39.160	10.410	32.662	1.00	21.13	7
ATOM	2197	C	ASN	A	266	37.441	12.394	30.944	1.00	13.73	6
ATOM	2198	O	ASN	A	266	37.161	13.123	31.927	1.00	13.68	8
ATOM	2199	N	ALA	A	267	36.552	11.545	30.362	1.00	13.47	7
ATOM	2200	CA	ALA	A	267	35.178	11.440	30.835	1.00	13.35	6
ATOM	2201	CB	ALA	A	267	34.330	10.522	29.944	1.00	12.56	6
ATOM	2202	C	ALA	A	267	35.076	10.997	32.287	1.00	13.08	6
ATOM	2203	O	ALA	A	267	34.195	11.454	33.027	1.00	13.14	8
ATOM	2204	N	GLY	A	268	35.918	10.106	32.733	1.00	12.97	7
ATOM	2205	CA	GLY	A	268	35.973	9.564	34.083	1.00	12.93	6
ATOM	2206	C	GLY	A	268	36.184	10.653	35.146	1.00	13.05	6
ATOM	2207	O	GLY	A	268	35.512	10.656	36.213	1.00	13.01	8
ATOM	2208	N	LYS	A	269	37.109	11.575	34.879	1.00	12.90	7
ATOM	2209	CA	LYS	A	269	37.425	12.681	35.786	1.00	13.04	6
ATOM	2210	CB	LYS	A	269	38.790	13.296	35.417	1.00	17.83	6
ATOM	2211	CG	LYS	A	269	39.840	12.506	36.217	1.00	22.85	6
ATOM	2212	CD	LYS	A	269	40.869	12.034	35.211	1.00	27.74	6
ATOM	2213	CE	LYS	A	269	41.722	10.885	35.785	1.00	30.85	6
ATOM	2214	NZ	LYS	A	269	42.663	10.356	34.698	1.00	32.23	7
ATOM	2215	C	LYS	A	269	36.296	13.699	35.776	1.00	12.76	6
ATOM	2216	O	LYS	A	269	35.918	14.230	36.828	1.00	12.65	8
ATOM	2217	N	LEU	A	270	35.696	13.903	34.596	1.00	12.42	7
ATOM	2218	CA	LEU	A	270	34.539	14.810	34.538	1.00	12.16	6
ATOM	2219	CB	LEU	A	270	34.164	15.161	33.088	1.00	13.49	6
ATOM	2220	CG	LEU	A	270	34.959	16.348	32.467	1.00	13.12	6
ATOM	2221	CD1	LEU	A	270	34.614	17.623	33.197	1.00	13.42	6
ATOM	2222	CD2	LEU	A	270	36.465	16.210	32.550	1.00	13.72	6
ATOM	2223	C	LEU	A	270	33.412	14.169	35.315	1.00	11.76	6
ATOM	2224	O	LEU	A	270	32.700	14.934	35.981	1.00	11.63	8
ATOM	2225	N	GLU	A	271	33.219	12.851	35.281	1.00	11.41	7
ATOM	2226	CA	GLU	A	271	32.136	12.233	36.051	1.00	11.29	6

ATOM	2227	CB	GLU	A	271	32.024	10.817	35.510	1.00	16.08	6
ATOM	2228	CG	GLU	A	271	31.015	10.010	36.333	1.00	23.09	6
ATOM	2229	CD	GLU	A	271	30.861	8.627	35.720	1.00	27.19	6
ATOM	2230	OE1	GLU	A	271	29.716	8.351	35.359	1.00	29.23	8
ATOM	2231	OE2	GLU	A	271	31.830	7.845	35.526	1.00	30.01	8
ATOM	2232	C	GLU	A	271	32.339	12.279	37.554	1.00	10.89	6
ATOM	2233	O	GLU	A	271	31.458	12.370	38.404	1.00	10.58	8
ATOM	2234	N	ASN	A	272	33.615	12.189	37.987	1.00	10.66	7
ATOM	2235	CA	ASN	A	272	34.008	12.309	39.385	1.00	10.31	6
ATOM	2236	CB	ASN	A	272	35.520	12.089	39.643	1.00	11.32	6
ATOM	2237	CG	ASN	A	272	35.969	12.380	41.064	1.00	11.99	6
ATOM	2238	OD1	ASN	A	272	35.616	11.603	41.966	1.00	11.66	8
ATOM	2239	ND2	ASN	A	272	36.701	13.474	41.322	1.00	12.45	7
ATOM	2240	C	ASN	A	272	33.588	13.709	39.873	1.00	9.78	6
ATOM	2241	O	ASN	A	272	33.080	13.897	40.979	1.00	9.63	8
ATOM	2242	N	TYR	A	273	33.777	14.748	39.063	1.00	9.45	7
ATOM	2243	CA	TYR	A	273	33.349	16.104	39.486	1.00	9.06	6
ATOM	2244	CB	TYR	A	273	33.908	17.179	38.558	1.00	8.65	6
ATOM	2245	CG	TYR	A	273	33.509	18.626	38.903	1.00	8.44	6
ATOM	2246	CD1	TYR	A	273	34.242	19.333	39.838	1.00	8.51	6
ATOM	2247	CE1	TYR	A	273	33.915	20.650	40.228	1.00	8.39	6
ATOM	2248	CD2	TYR	A	273	32.391	19.231	38.364	1.00	8.33	6
ATOM	2249	CE2	TYR	A	273	32.015	20.523	38.695	1.00	8.66	6
ATOM	2250	CZ	TYR	A	273	32.827	21.214	39.625	1.00	8.60	6
ATOM	2251	OH	TYR	A	273	32.452	22.481	39.938	1.00	8.94	8
ATOM	2252	C	TYR	A	273	31.837	16.135	39.662	1.00	9.06	6
ATOM	2253	O	TYR	A	273	31.340	16.679	40.688	1.00	8.80	8
ATOM	2254	N	LEU	A	274	31.061	15.569	38.736	1.00	9.52	7
ATOM	2255	CA	LEU	A	274	29.590	15.550	38.849	1.00	10.16	6
ATOM	2256	CB	LEU	A	274	28.901	14.856	37.646	1.00	10.22	6
ATOM	2257	CG	LEU	A	274	29.158	15.528	36.280	1.00	10.91	6
ATOM	2258	CD1	LEU	A	274	28.719	14.634	35.107	1.00	11.67	6
ATOM	2259	CD2	LEU	A	274	28.432	16.843	36.198	1.00	10.03	6
ATOM	2260	C	LEU	A	274	29.157	14.918	40.173	1.00	10.59	6
ATOM	2261	O	LEU	A	274	28.353	15.463	40.920	1.00	10.27	8
ATOM	2262	N	ASN	A	275	29.706	13.730	40.471	1.00	11.45	7
ATOM	2263	CA	ASN	A	275	29.463	13.009	41.709	1.00	12.37	6
ATOM	2264	CB	ASN	A	275	30.287	11.694	41.835	1.00	19.11	6
ATOM	2265	CG	ASN	A	275	29.761	10.565	40.962	1.00	24.07	6
ATOM	2266	OD1	ASN	A	275	28.743	9.915	41.314	1.00	27.53	8
ATOM	2267	ND2	ASN	A	275	30.352	10.254	39.805	1.00	25.40	7
ATOM	2268	C	ASN	A	275	29.820	13.870	42.924	1.00	12.34	6
ATOM	2269	O	ASN	A	275	28.964	14.072	43.761	1.00	12.19	8
ATOM	2270	N	LYS	A	276	31.008	14.435	43.005	1.00	12.51	7
ATOM	2271	CA	LYS	A	276	31.461	15.251	44.130	1.00	12.99	6
ATOM	2272	CB	LYS	A	276	32.952	15.605	44.000	1.00	12.82	6
ATOM	2273	CG	LYS	A	276	33.825	14.346	44.050	1.00	13.95	6
ATOM	2274	CD	LYS	A	276	33.535	13.485	45.269	1.00	14.29	6
ATOM	2275	CE	LYS	A	276	34.141	12.103	45.203	1.00	13.18	6
ATOM	2276	NZ	LYS	A	276	35.602	12.070	44.906	1.00	13.50	7
ATOM	2277	C	LYS	A	276	30.651	16.533	44.311	1.00	13.24	6
ATOM	2278	O	LYS	A	276	30.650	17.117	45.412	1.00	13.75	8
ATOM	2279	N	THR	A	277	29.966	16.979	43.256	1.00	12.99	7
ATOM	2280	CA	THR	A	277	29.173	18.187	43.406	1.00	12.78	6
ATOM	2281	CB	THR	A	277	29.520	19.264	42.357	1.00	12.02	6
ATOM	2282	OG1	THR	A	277	29.323	18.649	41.065	1.00	12.30	8
ATOM	2283	CG2	THR	A	277	30.941	19.791	42.492	1.00	8.90	6
ATOM	2284	C	THR	A	277	27.701	17.794	43.416	1.00	12.70	6
ATOM	2285	O	THR	A	277	26.812	18.613	43.190	1.00	12.66	8
ATOM	2286	N	SER	A	278	27.426	16.518	43.673	1.00	12.73	7
ATOM	2287	CA	SER	A	278	26.069	16.047	43.729	1.00	12.83	6
ATOM	2288	CB	SER	A	278	25.280	16.804	44.854	1.00	14.69	6
ATOM	2289	OG	SER	A	278	25.963	16.531	46.061	1.00	18.04	8
ATOM	2290	C	SER	A	278	25.283	16.294	42.474	1.00	12.85	6
ATOM	2291	O	SER	A	278	24.049	16.483	42.663	1.00	13.07	8
ATOM	2292	N	PHE	A	279	25.774	16.339	41.260	1.00	12.49	7
ATOM	2293	CA	PHE	A	279	24.897	16.593	40.100	1.00	12.16	6
ATOM	2294	CB	PHE	A	279	23.976	15.344	39.973	1.00	12.70	6
ATOM	2295	CG	PHE	A	279	24.772	14.122	39.524	1.00	12.87	6
ATOM	2296	CD1	PHE	A	279	25.183	13.153	40.435	1.00	13.85	6
ATOM	2297	CD2	PHE	A	279	25.085	13.919	38.199	1.00	13.30	6
ATOM	2298	CE1	PHE	A	279	25.903	12.038	40.045	1.00	13.14	6
ATOM	2299	CE2	PHE	A	279	25.801	12.799	37.786	1.00	13.99	6
ATOM	2300	CZ	PHE	A	279	26.246	11.878	38.726	1.00	13.30	6
ATOM	2301	C	PHE	A	279	24.170	17.912	40.149	1.00	12.03	6
ATOM	2302	O	PHE	A	279	23.185	18.072	39.417	1.00	12.27	8
ATOM	2303	N	ASN	A	280	24.646	18.942	40.882	1.00	11.58	7
ATOM	2304	CA	ASN	A	280	23.979	20.228	40.984	1.00	11.30	6
ATOM	2305	CB	ASN	A	280	24.025	20.735	42.438	1.00	11.18	6
ATOM	2306	CG	ASN	A	280	25.222	21.558	42.868	1.00	13.48	6
ATOM	2307	OD1	ASN	A	280	26.142	21.809	42.087	1.00	12.89	8
ATOM	2308	ND2	ASN	A	280	25.289	22.094	44.111	1.00	12.18	7
ATOM	2309	C	ASN	A	280	24.422	21.247	39.927	1.00	10.94	6
ATOM	2310	O	ASN	A	280	23.910	22.353	39.820	1.00	11.03	8
ATOM	2311	N	GLN	A	281	25.325	20.890	39.032	1.00	10.60	7
ATOM	2312	CA	GLN	A	281	25.784	21.736	37.949	1.00	10.04	6
ATOM	2313	CB	GLN	A	281	26.930	22.636	38.400	1.00	9.98	6
ATOM	2314	CG	GLN	A	281	28.117	21.977	39.038	1.00	9.72	6
ATOM	2315	CD	GLN	A	281	29.055	22.863	39.859	1.00	9.00	6
ATOM	2316	OE1	GLN	A	281	30.064	23.342	39.350	1.00	8.97	8
ATOM	2317	NE2	GLN	A	281	28.835	23.085	41.151	1.00	8.05	7
ATOM	2318	C	GLN	A	281	26.239	20.871	36.771	1.00	9.46	6
ATOM	2319	O	GLN	A	281	26.615	19.703	36.902	1.00	9.22	8
ATOM	2320	N	SER	A	282	26.224	21.522	35.616	1.00	9.14	7
ATOM	2321	CA	SER	A	282	26.674	20.851	34.389	1.00	8.74	6
ATOM	2322	CB	SER	A	282	25.985	21.419	33.131	1.00	7.22	6
ATOM	2323	OG	SER	A	282	24.607	21.123	33.102	1.00	6.53	8
ATOM	2324	C	SER	A	282	28.170	21.077	34.201	1.00	8.54	6
ATOM	2325	O	SER	A	282	28.773	21.913	34.919	1.00	8.89	8
ATOM	2326	N	VAL	A	283	28.777	20.420	33.240	1.00	8.11	7
ATOM	2327	CA	VAL	A	283	30.154	20.596	32.841	1.00	7.98	6
ATOM	2328	CB	VAL	A	283	31.137	19.443	33.210	1.00	8.54	6
ATOM	2329	CG1	VAL	A	283	31.457	19.441	34.708	1.00	9.20	6
ATOM	2330	CG2	VAL	A	283	30.599	18.117	32.719	1.00	7.85	6
ATOM	2331	C	VAL	A	283	30.218	20.758	31.304	1.00	7.87	6
ATOM	2332	O	VAL	A	283	29.342	20.265	30.572	1.00	7.75	8

ATOM	2333	N	PHE	A	284	31.212	21.483	30.801	1.00	7.72	7
ATOM	2334	CA	PHE	A	284	31.460	21.589	29.383	1.00	7.67	6
ATOM	2335	CB	PHE	A	284	32.518	22.649	29.110	1.00	7.48	6
ATOM	2336	CG	PHE	A	284	31.953	24.040	29.240	1.00	7.61	6
ATOM	2337	CD1	PHE	A	284	32.301	24.886	30.277	1.00	6.90	6
ATOM	2338	CD2	PHE	A	284	31.062	24.475	28.252	1.00	7.80	6
ATOM	2339	CE1	PHE	A	284	31.782	26.167	30.312	1.00	8.33	6
ATOM	2340	CE2	PHE	A	284	30.501	25.756	28.282	1.00	6.48	6
ATOM	2341	CZ	PHE	A	284	30.882	26.602	29.314	1.00	7.74	6
ATOM	2342	C	PHE	A	284	31.997	20.212	28.924	1.00	7.86	6
ATOM	2343	O	PHE	A	284	32.833	19.541	29.627	1.00	7.52	8
ATOM	2344	N	ASP	A	285	31.517	19.758	27.741	1.00	7.99	7
ATOM	2345	CA	ASP	A	285	31.997	18.452	27.212	1.00	8.11	6
ATOM	2346	CB	ASP	A	285	30.919	17.867	26.269	1.00	8.64	6
ATOM	2347	CG	ASP	A	285	31.063	16.361	26.096	1.00	9.93	6
ATOM	2348	OD1	ASP	A	285	32.173	15.774	26.289	1.00	8.07	8
ATOM	2349	OD2	ASP	A	285	30.026	15.731	25.769	1.00	9.24	8
ATOM	2350	C	ASP	A	285	33.339	18.591	26.496	1.00	8.25	6
ATOM	2351	O	ASP	A	285	33.394	18.729	25.236	1.00	8.58	8
ATOM	2352	N	VAL	A	286	34.468	18.590	27.218	1.00	7.95	7
ATOM	2353	CA	VAL	A	286	35.813	18.709	26.644	1.00	7.75	6
ATOM	2354	CB	VAL	A	286	36.851	18.934	27.764	1.00	7.80	6
ATOM	2355	CG1	VAL	A	286	38.270	19.085	27.261	1.00	5.55	6
ATOM	2356	CG2	VAL	A	286	36.418	20.221	28.524	1.00	8.40	6
ATOM	2357	C	VAL	A	286	36.145	17.549	25.719	1.00	7.74	6
ATOM	2358	O	VAL	A	286	36.611	17.833	24.601	1.00	7.94	8
ATOM	2359	N	PRO	A	287	35.967	16.276	26.097	1.00	7.41	7
ATOM	2360	CD	PRO	A	287	35.495	15.854	27.413	1.00	7.11	6
ATOM	2361	CA	PRO	A	287	36.262	15.131	25.226	1.00	7.24	6
ATOM	2362	CB	PRO	A	287	35.802	13.885	25.970	1.00	7.14	6
ATOM	2363	CG	PRO	A	287	35.741	14.357	27.396	1.00	7.12	6
ATOM	2364	C	PRO	A	287	35.589	15.313	23.873	1.00	7.43	6
ATOM	2365	O	PRO	A	287	36.214	15.113	22.834	1.00	7.51	8
ATOM	2366	N	LEU	A	288	34.293	15.681	23.762	1.00	7.47	7
ATOM	2367	CA	LEU	A	288	33.608	15.904	22.504	1.00	7.34	6
ATOM	2368	CB	LEU	A	288	32.149	16.325	22.654	1.00	7.25	6
ATOM	2369	CG	LEU	A	288	31.430	16.481	21.283	1.00	8.35	6
ATOM	2370	CD1	LEU	A	288	31.384	15.185	20.494	1.00	8.34	6
ATOM	2371	CD2	LEU	A	288	30.038	16.988	21.510	1.00	5.28	6
ATOM	2372	C	LEU	A	288	34.329	16.998	21.722	1.00	7.39	6
ATOM	2373	O	LEU	A	288	34.398	16.793	20.525	1.00	7.49	8
ATOM	2374	N	HIS	A	289	34.847	18.097	22.260	1.00	7.34	7
ATOM	2375	CA	HIS	A	289	35.583	19.114	21.525	1.00	7.21	6
ATOM	2376	CB	HIS	A	289	36.094	20.260	22.445	1.00	5.61	6
ATOM	2377	CG	HIS	A	289	37.215	21.083	21.852	1.00	5.00	6
ATOM	2378	CD2	HIS	A	289	38.548	21.040	22.012	1.00	5.00	6
ATOM	2379	ND1	HIS	A	289	36.986	22.086	20.914	1.00	5.00	7
ATOM	2380	CE1	HIS	A	289	38.127	22.570	20.527	1.00	5.00	6
ATOM	2381	NE2	HIS	A	289	39.124	21.983	21.176	1.00	5.00	7
ATOM	2382	C	HIS	A	289	36.776	18.507	20.805	1.00	7.52	6
ATOM	2383	O	HIS	A	289	37.083	18.809	19.647	1.00	7.41	8
ATOM	2384	N	PHE	A	290	37.518	17.654	21.545	1.00	7.75	7
ATOM	2385	CA	PHE	A	290	38.721	16.971	21.050	1.00	8.12	6
ATOM	2386	CB	PHE	A	290	39.575	16.332	22.175	1.00	7.08	6
ATOM	2387	CG	PHE	A	290	40.370	17.378	22.893	1.00	7.95	6
ATOM	2388	CD1	PHE	A	290	40.054	17.819	24.152	1.00	7.13	6
ATOM	2389	CD2	PHE	A	290	41.431	18.012	22.214	1.00	9.46	6
ATOM	2390	CE1	PHE	A	290	40.764	18.810	24.791	1.00	8.24	6
ATOM	2391	CE2	PHE	A	290	42.137	19.075	22.838	1.00	9.38	6
ATOM	2392	CZ	PHE	A	290	41.830	19.458	24.125	1.00	9.13	6
ATOM	2393	C	PHE	A	290	38.361	15.943	19.984	1.00	8.42	6
ATOM	2394	O	PHE	A	290	39.158	15.881	19.025	1.00	8.61	8
ATOM	2395	N	ASN	A	291	37.239	15.234	20.127	1.00	8.43	7
ATOM	2396	CA	ASN	A	291	36.826	14.303	19.077	1.00	8.66	6
ATOM	2397	CB	ASN	A	291	35.581	13.461	19.414	1.00	9.01	6
ATOM	2398	CG	ASN	A	291	35.866	12.427	20.505	1.00	10.93	6
ATOM	2399	OD1	ASN	A	291	37.040	12.332	20.954	1.00	10.93	8
ATOM	2400	ND2	ASN	A	291	34.848	11.690	20.917	1.00	8.51	7
ATOM	2401	C	ASN	A	291	36.507	15.080	17.798	1.00	8.93	6
ATOM	2402	O	ASN	A	291	36.824	14.630	16.701	1.00	8.32	8
ATOM	2403	N	LEU	A	292	35.808	16.219	17.925	1.00	9.66	7
ATOM	2404	CA	LEU	A	292	35.459	17.043	16.777	1.00	10.78	6
ATOM	2405	CB	LEU	A	292	34.525	18.220	17.143	1.00	11.55	6
ATOM	2406	CG	LEU	A	292	33.126	17.717	17.616	1.00	12.98	6
ATOM	2407	CD1	LEU	A	292	32.406	18.847	18.358	1.00	10.98	6
ATOM	2408	CD2	LEU	A	292	32.371	17.124	16.439	1.00	11.27	6
ATOM	2409	C	LEU	A	292	36.713	17.628	16.088	1.00	11.19	6
ATOM	2410	O	LEU	A	292	36.821	17.685	14.878	1.00	11.27	8
ATOM	2411	N	GLN	A	293	37.674	18.093	16.832	1.00	11.50	7
ATOM	2412	CA	GLN	A	293	38.899	18.619	16.322	1.00	12.28	6
ATOM	2413	CB	GLN	A	293	39.632	19.090	17.572	1.00	15.35	6
ATOM	2414	CG	GLN	A	293	40.644	20.159	17.294	1.00	20.28	6
ATOM	2415	CD	GLN	A	293	42.018	19.550	17.111	1.00	23.63	6
ATOM	2416	OE1	GLN	A	293	42.277	18.617	17.883	1.00	27.19	8
ATOM	2417	NE2	GLN	A	293	42.755	20.086	16.154	1.00	25.26	7
ATOM	2418	C	GLN	A	293	39.771	17.574	15.581	1.00	12.47	6
ATOM	2419	O	GLN	A	293	40.424	17.827	14.578	1.00	12.05	8
ATOM	2420	N	ALA	A	294	39.793	16.376	16.196	1.00	12.83	7
ATOM	2421	CA	ALA	A	294	40.557	15.278	15.655	1.00	13.37	6
ATOM	2422	CB	ALA	A	294	40.630	14.069	16.583	1.00	12.51	6
ATOM	2423	C	ALA	A	294	39.920	14.904	14.299	1.00	13.89	6
ATOM	2424	O	ALA	A	294	40.681	14.764	13.312	1.00	14.17	8
ATOM	2425	N	ALA	A	295	38.580	14.804	14.185	1.00	13.85	7
ATOM	2426	CA	ALA	A	295	37.963	14.486	12.906	1.00	13.85	6
ATOM	2427	CB	ALA	A	295	36.447	14.351	12.963	1.00	11.81	6
ATOM	2428	C	ALA	A	295	38.280	15.584	11.874	1.00	14.11	6
ATOM	2429	O	ALA	A	295	38.474	15.301	10.678	1.00	14.15	8
ATOM	2430	N	SER	A	296	38.311	16.845	12.322	1.00	14.00	7
ATOM	2431	CA	SER	A	296	38.562	17.954	11.422	1.00	14.17	6
ATOM	2432	CB	SER	A	296	38.176	19.248	12.167	1.00	10.42	6
ATOM	2433	OG	SER	A	296	39.176	19.868	12.880	1.00	8.51	8
ATOM	2434	C	SER	A	296	40.000	17.997	10.859	1.00	14.43	6
ATOM	2435	O	SER	A	296	40.338	18.622	9.838	1.00	14.12	8
ATOM	2436	N	SER	A	297	40.902	17.322	11.540	1.00	14.82	7
ATOM	2437	CA	SER	A	297	42.305	17.287	11.269	1.00	15.50	6
ATOM	2438	CB	SER	A	297	42.931	16.991	12.708	1.00	16.67	6

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ATOM	2439	OG	SER	A	297	42.921	18.303	13.176	1.00	20.24	8
ATOM	2440	C	SER	A	297	42.921	16.146	10.508	1.00	15.90	6
ATOM	2441	O	SER	A	297	44.076	16.216	10.160	1.00	15.87	8
ATOM	2442	N	GLN	A	298	42.143	15.074	10.370	1.00	16.33	7
ATOM	2443	CA	GLN	A	298	42.650	13.888	9.722	1.00	16.82	6
ATOM	2444	CB	GLN	A	298	42.156	12.653	10.523	1.00	18.92	6
ATOM	2445	CG	GLN	A	298	43.084	12.447	11.693	1.00	20.51	6
ATOM	2446	CD	GLN	A	298	42.613	11.548	12.798	1.00	23.02	6
ATOM	2447	OE1	GLN	A	298	42.174	10.410	12.588	1.00	24.09	8
ATOM	2448	NE2	GLN	A	298	42.715	12.077	14.034	1.00	23.74	7
ATOM	2449	C	GLN	A	298	42.319	13.823	8.245	1.00	17.02	6
ATOM	2450	O	GLN	A	298	42.486	12.719	7.679	1.00	17.29	8
ATOM	2451	N	GLY	A	299	41.907	14.913	7.631	1.00	16.90	7
ATOM	2452	CA	GLY	A	299	41.595	15.001	6.223	1.00	16.90	6
ATOM	2453	C	GLY	A	299	40.763	13.864	5.685	1.00	16.77	6
ATOM	2454	O	GLY	A	299	40.942	13.480	4.523	1.00	17.33	8
ATOM	2455	N	GLY	A	300	39.855	13.274	6.435	1.00	16.11	7
ATOM	2456	CA	GLY	A	300	39.068	12.163	5.983	1.00	15.25	6
ATOM	2457	C	GLY	A	300	39.483	10.868	6.650	1.00	14.82	6
ATOM	2458	O	GLY	A	300	38.603	10.027	6.489	1.00	14.53	8
ATOM	2459	N	GLY	A	301	40.574	10.532	7.302	1.00	14.47	7
ATOM	2460	CA	GLY	A	301	40.815	9.227	7.860	1.00	14.37	6
ATOM	2461	C	GLY	A	301	40.234	8.948	9.225	1.00	14.36	6
ATOM	2462	O	GLY	A	301	40.318	7.830	9.696	1.00	14.17	8
ATOM	2463	N	TYR	A	302	39.559	9.888	9.908	1.00	14.62	7
ATOM	2464	CA	TYR	A	302	38.973	9.650	11.220	1.00	14.57	6
ATOM	2465	CB	TYR	A	302	38.419	10.956	11.845	1.00	14.59	6
ATOM	2466	CG	TYR	A	302	37.750	10.869	13.198	1.00	14.61	6
ATOM	2467	CD1	TYR	A	302	38.559	10.860	14.355	1.00	14.96	6
ATOM	2468	CE1	TYR	A	302	37.990	10.754	15.630	1.00	14.98	6
ATOM	2469	CD2	TYR	A	302	36.380	10.751	13.400	1.00	14.40	6
ATOM	2470	CE2	TYR	A	302	35.820	10.629	14.663	1.00	14.56	6
ATOM	2471	CZ	TYR	A	302	36.622	10.655	15.778	1.00	14.83	6
ATOM	2472	OH	TYR	A	302	36.157	10.564	17.049	1.00	15.01	8
ATOM	2473	C	TYR	A	302	37.831	8.643	11.151	1.00	14.74	6
ATOM	2474	O	TYR	A	302	37.073	8.682	10.170	1.00	14.62	8
ATOM	2475	N	ASP	A	303	37.515	7.744	12.058	1.00	14.71	7
ATOM	2476	CA	ASP	A	303	36.350	6.873	11.910	1.00	14.90	6
ATOM	2477	CB	ASP	A	303	36.617	5.550	12.620	1.00	16.31	6
ATOM	2478	CG	ASP	A	303	35.526	4.517	12.403	1.00	17.88	6
ATOM	2479	OD1	ASP	A	303	34.383	4.796	12.005	1.00	17.07	8
ATOM	2480	OD2	ASP	A	303	35.893	3.348	12.637	1.00	19.55	8
ATOM	2481	C	ASP	A	303	35.165	7.627	12.500	1.00	14.85	6
ATOM	2482	O	ASP	A	303	35.013	7.729	13.714	1.00	14.59	8
ATOM	2483	N	MET	A	304	34.315	8.199	11.658	1.00	14.94	7
ATOM	2484	CA	MET	A	304	33.151	8.973	12.057	1.00	15.29	6
ATOM	2485	CB	MET	A	304	32.440	9.630	10.862	1.00	14.35	6
ATOM	2486	CG	MET	A	304	33.307	10.718	10.201	1.00	13.91	6
ATOM	2487	SD	MET	A	304	33.391	12.309	11.028	1.00	14.76	16
ATOM	2488	CE	MET	A	304	31.941	13.156	10.378	1.00	11.94	6
ATOM	2489	C	MET	A	304	32.161	8.195	12.917	1.00	15.60	6
ATOM	2490	O	MET	A	304	31.322	8.846	13.549	1.00	15.54	8
ATOM	2491	N	ARG	A	305	32.251	6.872	13.019	1.00	15.77	7
ATOM	2492	CA	ARG	A	305	31.372	6.123	13.883	1.00	16.15	6
ATOM	2493	CB	ARG	A	305	31.398	4.601	13.558	1.00	17.94	6
ATOM	2494	CG	ARG	A	305	30.663	4.270	12.266	1.00	20.53	6
ATOM	2495	CD	ARG	A	305	30.984	3.018	11.512	1.00	21.54	6
ATOM	2496	NE	ARG	A	305	32.390	2.813	11.326	1.00	23.87	7
ATOM	2497	CZ	ARG	A	305	32.917	1.717	10.819	1.00	26.93	6
ATOM	2498	NH1	ARG	A	305	32.145	0.716	10.412	1.00	29.01	7
ATOM	2499	NH2	ARG	A	305	34.239	1.652	10.753	1.00	28.19	7
ATOM	2500	C	ARG	A	305	31.768	6.318	15.354	1.00	16.33	6
ATOM	2501	O	ARG	A	305	30.997	5.924	16.218	1.00	16.15	8
ATOM	2502	N	LYS	A	306	32.942	6.837	15.661	1.00	16.51	7
ATOM	2503	CA	LYS	A	306	33.424	7.006	17.011	1.00	17.04	6
ATOM	2504	CB	LYS	A	306	34.945	6.643	16.903	1.00	19.89	6
ATOM	2505	CG	LYS	A	306	35.043	5.174	16.504	1.00	25.08	6
ATOM	2506	CD	LYS	A	306	36.487	4.726	16.705	1.00	30.20	6
ATOM	2507	CE	LYS	A	306	36.968	3.663	15.712	1.00	32.87	6
ATOM	2508	NZ	LYS	A	306	37.911	2.695	16.442	1.00	35.11	7
ATOM	2509	C	LYS	A	306	33.356	8.375	17.653	1.00	17.07	6
ATOM	2510	O	LYS	A	306	33.967	8.639	18.692	1.00	16.98	8
ATOM	2511	N	LEU	A	307	32.639	9.313	17.026	1.00	17.11	7
ATOM	2512	CA	LEU	A	307	32.539	10.700	17.444	1.00	17.21	6
ATOM	2513	CB	LEU	A	307	31.608	11.509	16.526	1.00	18.35	6
ATOM	2514	CG	LEU	A	307	32.192	12.263	15.348	1.00	20.88	6
ATOM	2515	CD1	LEU	A	307	31.055	12.963	14.582	1.00	21.03	6
ATOM	2516	CD2	LEU	A	307	33.273	13.283	15.684	1.00	20.35	6
ATOM	2517	C	LEU	A	307	32.084	10.826	18.890	1.00	17.01	6
ATOM	2518	O	LEU	A	307	32.553	11.677	19.605	1.00	17.09	8
ATOM	2519	N	LEU	A	308	31.179	9.970	19.331	1.00	16.89	7
ATOM	2520	CA	LEU	A	308	30.629	9.973	20.670	1.00	16.75	6
ATOM	2521	CB	LEU	A	308	29.153	9.440	20.589	1.00	17.24	6
ATOM	2522	CG	LEU	A	308	28.116	10.476	20.136	1.00	19.15	6
ATOM	2523	CD1	LEU	A	308	26.740	9.862	19.977	1.00	18.81	6
ATOM	2524	CD2	LEU	A	308	28.015	11.685	21.063	1.00	19.79	6
ATOM	2525	C	LEU	A	308	31.420	9.200	21.720	1.00	16.38	6
ATOM	2526	O	LEU	A	308	31.137	9.327	22.922	1.00	16.30	8
ATOM	2527	N	ASN	A	309	32.381	8.386	21.344	1.00	16.16	7
ATOM	2528	CA	ASN	A	309	33.203	7.595	22.228	1.00	15.89	6
ATOM	2529	CB	ASN	A	309	34.349	6.886	21.492	1.00	21.07	6
ATOM	2530	CG	ASN	A	309	33.880	5.720	20.660	1.00	26.35	6
ATOM	2531	OD1	ASN	A	309	34.746	5.049	20.024	1.00	29.82	8
ATOM	2532	ND2	ASN	A	309	32.579	5.435	20.588	1.00	27.51	7
ATOM	2533	C	ASN	A	309	33.938	8.456	23.265	1.00	15.16	6
ATOM	2534	O	ASN	A	309	34.623	9.384	22.831	1.00	15.00	8
ATOM	2535	N	GLY	A	310	33.777	8.102	24.545	1.00	14.32	7
ATOM	2536	CA	GLY	A	310	34.447	8.836	25.603	1.00	13.49	6
ATOM	2537	C	GLY	A	310	33.944	10.232	25.938	1.00	12.69	6
ATOM	2538	O	GLY	A	310	34.667	10.890	26.657	1.00	12.41	8
ATOM	2539	N	THR	A	311	32.784	10.615	25.413	1.00	12.19	7
ATOM	2540	CA	THR	A	311	32.222	11.929	25.676	1.00	11.65	6
ATOM	2541	CB	THR	A	311	31.462	12.519	24.452	1.00	10.26	6
ATOM	2542	OG1	THR	A	311	30.315	11.692	24.240	1.00	10.86	8
ATOM	2543	CG2	THR	A	311	32.307	12.571	23.191	1.00	8.42	6
ATOM	2544	C	THR	A	311	31.284	11.908	26.895	1.00	11.36	6

ATOM	2545	O	THR	A	311	30.667	10.902	27.258	1.00 11.29	8
ATOM	2546	N	VAL	A	312	31.198	13.075	27.545	1.00 11.20	7
ATOM	2547	CA	VAL	A	312	30.313	13.282	28.693	1.00 11.29	6
ATOM	2548	CB	VAL	A	312	30.567	14.637	29.407	1.00 12.62	6
ATOM	2549	CG1	VAL	A	312	29.620	14.906	30.597	1.00 13.45	6
ATOM	2550	CG2	VAL	A	312	31.995	14.730	29.912	1.00 10.56	6
ATOM	2551	C	VAL	A	312	28.874	13.189	28.191	1.00 11.23	6
ATOM	2552	O	VAL	A	312	28.053	12.526	28.793	1.00 11.01	8
ATOM	2553	N	VAL	A	313	28.533	13.825	27.061	1.00 11.42	7
ATOM	2554	CA	VAL	A	313	27.208	13.790	26.498	1.00 11.94	6
ATOM	2555	CB	VAL	A	313	27.107	14.723	25.266	1.00 12.88	6
ATOM	2556	CG1	VAL	A	313	27.604	14.175	23.942	1.00 13.11	6
ATOM	2557	CG2	VAL	A	313	25.627	15.102	25.100	1.00 14.06	6
ATOM	2558	C	VAL	A	313	26.655	12.380	26.219	1.00 12.21	6
ATOM	2559	O	VAL	A	313	25.434	12.216	26.319	1.00 11.69	8
ATOM	2560	N	SER	A	314	27.418	11.313	25.971	1.00 12.83	7
ATOM	2561	CA	SER	A	314	26.878	9.987	25.750	1.00 13.56	6
ATOM	2562	CB	SER	A	314	27.801	9.054	24.922	1.00 13.63	6
ATOM	2563	OG	SER	A	314	29.056	9.048	25.641	1.00 15.90	8
ATOM	2564	C	SER	A	314	26.572	9.345	27.111	1.00 14.04	6
ATOM	2565	O	SER	A	314	25.730	8.445	27.105	1.00 14.28	8
ATOM	2566	N	LYS	A	315	27.168	9.725	28.254	1.00 14.23	7
ATOM	2567	CA	LYS	A	315	26.823	9.081	29.513	1.00 14.22	6
ATOM	2568	CB	LYS	A	315	27.928	8.797	30.491	1.00 19.81	6
ATOM	2569	CG	LYS	A	315	29.333	8.495	30.319	1.00 26.75	6
ATOM	2570	CD	LYS	A	315	30.321	9.661	30.402	1.00 32.49	6
ATOM	2571	CE	LYS	A	315	30.714	10.114	31.825	1.00 35.30	6
ATOM	2572	NZ	LYS	A	315	31.599	9.199	32.634	1.00 35.57	7
ATOM	2573	C	LYS	A	315	25.884	9.951	30.379	1.00 13.74	6
ATOM	2574	O	LYS	A	315	24.969	9.435	31.020	1.00 13.60	8
ATOM	2575	N	HIS	A	316	26.108	11.257	30.397	1.00 13.12	7
ATOM	2576	CA	HIS	A	316	25.314	12.197	31.179	1.00 13.02	6
ATOM	2577	CB	HIS	A	316	26.202	12.791	32.327	1.00 12.69	6
ATOM	2578	CG	HIS	A	316	26.550	11.718	33.313	1.00 12.94	6
ATOM	2579	CD2	HIS	A	316	25.796	11.024	34.166	1.00 13.25	6
ATOM	2580	ND1	HIS	A	316	27.835	11.194	33.424	1.00 15.42	7
ATOM	2581	CE1	HIS	A	316	27.850	10.206	34.317	1.00 14.97	6
ATOM	2582	NE2	HIS	A	316	26.617	10.106	34.822	1.00 15.47	7
ATOM	2583	C	HIS	A	316	24.809	13.360	30.325	1.00 12.64	6
ATOM	2584	O	HIS	A	316	25.304	14.479	30.471	1.00 12.29	8
ATOM	2585	N	PRO	A	317	23.868	13.075	29.435	1.00 12.52	7
ATOM	2586	CD	PRO	A	317	23.256	11.740	29.268	1.00 12.43	6
ATOM	2587	CA	PRO	A	317	23.311	14.040	28.519	1.00 12.50	6
ATOM	2588	CB	PRO	A	317	22.280	13.268	27.640	1.00 12.54	6
ATOM	2589	CG	PRO	A	317	21.996	12.051	28.524	1.00 12.55	6
ATOM	2590	C	PRO	A	317	22.669	15.253	29.133	1.00 12.59	6
ATOM	2591	O	PRO	A	317	22.750	16.349	28.542	1.00 12.88	8
ATOM	2592	N	LEU	A	318	22.033	15.168	30.285	1.00 12.44	7
ATOM	2593	CA	LEU	A	318	21.370	16.286	30.956	1.00 12.38	6
ATOM	2594	CB	LEU	A	318	20.278	15.805	31.970	1.00 13.77	6
ATOM	2595	CG	LEU	A	318	19.256	14.834	31.334	1.00 15.85	6
ATOM	2596	CD1	LEU	A	318	18.250	14.143	32.241	1.00 15.19	6
ATOM	2597	CD2	LEU	A	318	18.520	15.629	30.254	1.00 17.19	6
ATOM	2598	C	LEU	A	318	22.338	17.175	31.741	1.00 11.91	6
ATOM	2599	O	LEU	A	318	21.929	18.174	32.286	1.00 11.51	8
ATOM	2600	N	LYS	A	319	23.602	16.757	31.836	1.00 11.53	7
ATOM	2601	CA	LYS	A	319	24.559	17.559	32.591	1.00 11.24	6
ATOM	2602	CB	LYS	A	319	25.135	16.758	33.794	1.00 12.25	6
ATOM	2603	CG	LYS	A	319	24.001	16.369	34.812	1.00 12.23	6
ATOM	2604	CD	LYS	A	319	23.655	17.705	35.470	1.00 13.91	6
ATOM	2605	CE	LYS	A	319	22.335	17.774	36.181	1.00 15.19	6
ATOM	2606	NZ	LYS	A	319	22.278	18.963	37.119	1.00 14.09	7
ATOM	2607	C	LYS	A	319	25.652	18.008	31.640	1.00 10.89	6
ATOM	2608	O	LYS	A	319	26.717	18.376	32.153	1.00 11.10	8
ATOM	2609	N	SER	A	320	25.462	17.969	30.320	1.00 10.24	7
ATOM	2610	CA	SER	A	320	26.564	18.409	29.483	1.00 9.74	6
ATOM	2611	CB	SER	A	320	26.825	17.443	28.311	1.00 11.44	6
ATOM	2612	OG	SER	A	320	26.960	16.158	28.752	1.00 15.00	8
ATOM	2613	C	SER	A	320	26.322	19.681	28.692	1.00 9.08	6
ATOM	2614	O	SER	A	320	25.215	19.672	28.144	1.00 9.21	8
ATOM	2615	N	VAL	A	321	27.294	20.549	28.581	1.00 8.35	7
ATOM	2616	CA	VAL	A	321	27.166	21.744	27.760	1.00 7.87	6
ATOM	2617	CB	VAL	A	321	27.455	23.085	28.447	1.00 6.55	6
ATOM	2618	CG1	VAL	A	321	27.468	24.283	27.473	1.00 5.70	6
ATOM	2619	CG2	VAL	A	321	26.352	23.381	29.489	1.00 6.25	6
ATOM	2620	C	VAL	A	321	28.079	21.422	26.585	1.00 7.79	6
ATOM	2621	O	VAL	A	321	29.282	21.146	26.791	1.00 8.06	8
ATOM	2622	N	THR	A	322	27.497	21.399	25.396	1.00 7.46	7
ATOM	2623	CA	THR	A	322	28.302	21.038	24.183	1.00 7.12	6
ATOM	2624	CB	THR	A	322	27.504	20.146	23.199	1.00 5.50	6
ATOM	2625	OG1	THR	A	322	26.184	20.559	22.923	1.00 5.00	8
ATOM	2626	CG2	THR	A	322	27.279	18.718	23.807	1.00 6.18	6
ATOM	2627	C	THR	A	322	28.877	22.262	23.492	1.00 7.07	6
ATOM	2628	O	THR	A	322	28.206	23.319	23.510	1.00 7.34	8
ATOM	2629	N	PHE	A	323	30.076	22.181	22.907	1.00 6.79	7
ATOM	2630	CA	PHE	A	323	30.734	23.301	22.257	1.00 6.58	6
ATOM	2631	CB	PHE	A	323	31.435	24.192	23.312	1.00 5.72	6
ATOM	2632	CG	PHE	A	323	32.752	23.783	23.849	1.00 5.21	6
ATOM	2633	CD1	PHE	A	323	33.918	24.279	23.270	1.00 6.61	6
ATOM	2634	CD2	PHE	A	323	32.864	22.861	24.884	1.00 6.77	6
ATOM	2635	CE1	PHE	A	323	35.167	23.880	23.764	1.00 7.34	6
ATOM	2636	CE2	PHE	A	323	34.105	22.368	25.363	1.00 6.08	6
ATOM	2637	CZ	PHE	A	323	35.238	22.944	24.795	1.00 6.00	6
ATOM	2638	C	PHE	A	323	31.727	22.855	21.184	1.00 6.75	6
ATOM	2639	O	PHE	A	323	32.313	21.743	21.207	1.00 6.74	8
ATOM	2640	N	VAL	A	324	31.917	23.744	20.208	1.00 6.84	7
ATOM	2641	CA	VAL	A	324	32.846	23.539	19.087	1.00 6.92	6
ATOM	2642	CB	VAL	A	324	32.248	24.084	17.759	1.00 6.12	6
ATOM	2643	CG1	VAL	A	324	33.175	23.923	16.595	1.00 5.00	6
ATOM	2644	CG2	VAL	A	324	30.945	23.335	17.428	1.00 5.00	6
ATOM	2645	C	VAL	A	324	34.230	24.137	19.434	1.00 7.23	6
ATOM	2646	O	VAL	A	324	35.247	23.410	19.508	1.00 6.91	8
ATOM	2647	N	ASP	A	325	34.276	25.479	19.678	1.00 7.39	7
ATOM	2648	CA	ASP	A	325	35.469	26.189	20.078	1.00 7.78	6
ATOM	2649	CB	ASP	A	325	36.180	26.898	18.918	1.00 8.62	6
ATOM	2650	CG	ASP	A	325	37.157	25.954	18.192	1.00 8.81	6

ATOM	2651	OD1	ASP	A	325	38.076	25.409	18.839	1.00	7.66	8
ATOM	2652	OD2	ASP	A	325	37.027	25.682	16.964	1.00	9.34	8
ATOM	2653	C	ASP	A	325	35.117	27.261	21.116	1.00	8.18	6
ATOM	2654	O	ASP	A	325	33.960	27.635	21.254	1.00	8.16	8
ATOM	2655	N	ASN	A	326	36.108	27.788	21.826	1.00	8.35	7
ATOM	2656	CA	ASN	A	326	35.925	28.845	22.813	1.00	8.28	6
ATOM	2657	CB	ASN	A	326	35.487	28.329	24.160	1.00	9.54	6
ATOM	2658	CG	ASN	A	326	36.502	27.485	24.902	1.00	11.91	6
ATOM	2659	OD1	ASN	A	326	37.701	27.415	24.622	1.00	12.52	8
ATOM	2660	ND2	ASN	A	326	36.121	26.782	25.965	1.00	11.95	7
ATOM	2661	C	ASN	A	326	37.212	29.685	22.871	1.00	8.44	6
ATOM	2662	O	ASN	A	326	38.140	29.601	22.053	1.00	7.98	8
ATOM	2663	N	HIS	A	327	37.266	30.626	23.836	1.00	8.65	7
ATOM	2664	CA	HIS	A	327	38.367	31.562	23.994	1.00	9.17	6
ATOM	2665	CB	HIS	A	327	37.976	32.718	24.999	1.00	8.48	6
ATOM	2666	CG	HIS	A	327	37.800	32.154	26.392	1.00	7.81	6
ATOM	2667	CD2	HIS	A	327	38.481	32.357	27.535	1.00	7.34	6
ATOM	2668	ND1	HIS	A	327	36.785	31.222	26.672	1.00	8.46	7
ATOM	2669	CE1	HIS	A	327	36.886	30.856	27.951	1.00	7.98	6
ATOM	2670	NE2	HIS	A	327	37.883	31.538	28.493	1.00	8.30	7
ATOM	2671	C	HIS	A	327	39.664	30.866	24.404	1.00	9.58	6
ATOM	2672	O	HIS	A	327	40.718	31.444	24.169	1.00	9.63	8
ATOM	2673	N	ASP	A	328	39.645	29.653	24.928	1.00	10.01	7
ATOM	2674	CA	ASP	A	328	40.783	28.869	25.312	1.00	10.53	6
ATOM	2675	CB	ASP	A	328	40.422	27.735	26.312	1.00	14.56	6
ATOM	2676	CG	ASP	A	328	39.676	27.936	27.629	1.00	18.50	6
ATOM	2677	OD1	ASP	A	328	40.162	28.843	28.385	1.00	17.22	8
ATOM	2678	OD2	ASP	A	328	38.615	27.265	28.055	1.00	18.97	8
ATOM	2679	C	ASP	A	328	41.385	28.188	24.074	1.00	10.65	6
ATOM	2680	O	ASP	A	328	42.607	28.041	23.933	1.00	10.58	8
ATOM	2681	N	THR	A	329	40.518	27.688	23.167	1.00	10.47	7
ATOM	2682	CA	THR	A	329	40.946	26.880	22.028	1.00	10.37	6
ATOM	2683	CB	THR	A	329	39.933	25.709	21.777	1.00	10.26	6
ATOM	2684	OG1	THR	A	329	38.709	26.293	21.286	1.00	9.63	8
ATOM	2685	CG2	THR	A	329	39.596	24.873	23.020	1.00	9.29	6
ATOM	2686	C	THR	A	329	41.142	27.596	20.702	1.00	10.36	6
ATOM	2687	O	THR	A	329	41.563	26.999	19.704	1.00	9.94	8
ATOM	2688	N	GLN	A	330	40.827	28.878	20.679	1.00	10.77	7
ATOM	2689	CA	GLN	A	330	40.985	29.688	19.441	1.00	11.30	6
ATOM	2690	CB	GLN	A	330	40.182	30.988	19.518	1.00	9.13	6
ATOM	2691	CG	GLN	A	330	40.749	31.987	20.543	1.00	8.40	6
ATOM	2692	CD	GLN	A	330	40.003	33.322	20.559	1.00	8.44	6
ATOM	2693	OE1	GLN	A	330	39.089	33.499	21.393	1.00	7.21	8
ATOM	2694	NE2	GLN	A	330	40.432	34.237	19.660	1.00	7.16	7
ATOM	2695	C	GLN	A	330	42.486	29.890	19.211	1.00	11.99	6
ATOM	2696	O	GLN	A	330	43.345	29.690	20.092	1.00	11.70	8
ATOM	2697	N	PRO	A	331	42.793	30.208	17.963	1.00	12.80	7
ATOM	2698	CD	PRO	A	331	41.806	30.403	16.873	1.00	12.95	6
ATOM	2699	CA	PRO	A	331	44.119	30.424	17.447	1.00	13.52	6
ATOM	2700	CB	PRO	A	331	43.974	30.918	15.966	1.00	13.53	6
ATOM	2701	CG	PRO	A	331	42.608	30.336	15.583	1.00	13.10	6
ATOM	2702	C	PRO	A	331	44.899	31.372	18.320	1.00	14.55	6
ATOM	2703	O	PRO	A	331	44.496	32.463	18.767	1.00	14.46	8
ATOM	2704	N	GLY	A	332	46.122	30.893	18.593	1.00	15.77	7
ATOM	2705	CA	GLY	A	332	47.087	31.624	19.404	1.00	17.06	6
ATOM	2706	C	GLY	A	332	46.881	31.463	20.896	1.00	18.22	6
ATOM	2707	O	GLY	A	332	47.755	31.915	21.633	1.00	18.26	8
ATOM	2708	N	GLN	A	333	45.817	30.862	21.429	1.00	19.06	7
ATOM	2709	CA	GLN	A	333	45.678	30.778	22.875	1.00	19.88	6
ATOM	2710	CB	GLN	A	333	44.181	30.838	23.241	1.00	19.70	6
ATOM	2711	CG	GLN	A	333	43.711	32.283	23.072	1.00	20.78	6
ATOM	2712	CD	GLN	A	333	44.572	33.254	23.876	1.00	23.47	6
ATOM	2713	OE1	GLN	A	333	45.181	34.191	23.315	1.00	26.12	8
ATOM	2714	NE2	GLN	A	333	44.705	33.056	25.175	1.00	22.30	7
ATOM	2715	C	GLN	A	333	46.462	29.622	23.446	1.00	20.87	6
ATOM	2716	O	GLN	A	333	47.167	28.850	22.773	1.00	20.84	8
ATOM	2717	N	SER	A	334	46.339	29.555	24.795	1.00	21.65	7
ATOM	2718	CA	SER	A	334	47.083	28.519	25.552	1.00	22.42	6
ATOM	2719	CB	SER	A	334	46.792	28.705	27.067	1.00	26.55	6
ATOM	2720	OG	SER	A	334	45.405	29.089	27.235	1.00	30.85	8
ATOM	2721	C	SER	A	334	46.790	27.074	25.194	1.00	22.23	6
ATOM	2722	O	SER	A	334	47.687	26.293	24.929	1.00	22.55	8
ATOM	2723	N	LEU	A	335	45.506	26.728	25.170	1.00	21.74	7
ATOM	2724	CA	LEU	A	335	44.958	25.411	24.863	1.00	20.75	6
ATOM	2725	CB	LEU	A	335	43.814	25.183	25.883	1.00	22.84	6
ATOM	2726	CG	LEU	A	335	44.252	25.266	27.365	1.00	23.70	6
ATOM	2727	CD1	LEU	A	335	43.065	25.292	28.305	1.00	23.07	6
ATOM	2728	CD2	LEU	A	335	45.184	24.089	27.673	1.00	24.51	6
ATOM	2729	C	LEU	A	335	44.460	25.313	23.427	1.00	19.68	6
ATOM	2730	O	LEU	A	335	43.491	24.609	23.136	1.00	19.77	8
ATOM	2731	N	GLU	A	336	45.111	26.053	22.536	1.00	18.47	7
ATOM	2732	CA	GLU	A	336	44.766	26.089	21.149	1.00	17.45	6
ATOM	2733	CB	GLU	A	336	45.908	26.773	20.387	1.00	19.49	6
ATOM	2734	CG	GLU	A	336	45.655	26.544	18.905	1.00	22.99	6
ATOM	2735	CD	GLU	A	336	46.508	27.440	18.036	1.00	26.38	6
ATOM	2736	OE1	GLU	A	336	47.378	28.166	18.504	1.00	26.94	8
ATOM	2737	OE2	GLU	A	336	46.276	27.487	16.805	1.00	28.18	8
ATOM	2738	C	GLU	A	336	44.504	24.698	20.571	1.00	16.40	6
ATOM	2739	O	GLU	A	336	45.349	23.802	20.647	1.00	16.09	8
ATOM	2740	N	SER	A	337	43.338	24.527	19.954	1.00	15.33	7
ATOM	2741	CA	SER	A	337	43.005	23.217	19.393	1.00	14.23	6
ATOM	2742	CB	SER	A	337	42.891	22.175	20.487	1.00	13.48	6
ATOM	2743	OG	SER	A	337	41.855	22.515	21.439	1.00	13.96	8
ATOM	2744	C	SER	A	337	41.679	23.436	18.645	1.00	13.82	6
ATOM	2745	O	SER	A	337	40.615	22.864	18.896	1.00	13.37	8
ATOM	2746	N	THR	A	338	41.878	24.333	17.679	1.00	13.53	7
ATOM	2747	CA	THR	A	338	40.800	24.801	16.837	1.00	13.46	6
ATOM	2748	CB	THR	A	338	41.340	26.036	16.033	1.00	13.02	6
ATOM	2749	OG1	THR	A	338	41.955	26.893	17.006	1.00	14.55	8
ATOM	2750	CG2	THR	A	338	40.259	26.794	15.338	1.00	12.29	6
ATOM	2751	C	THR	A	338	40.216	23.770	15.877	1.00	13.20	6
ATOM	2752	O	THR	A	338	40.980	23.008	15.281	1.00	13.26	8
ATOM	2753	N	VAL	A	339	38.905	23.766	15.743	1.00	12.73	7
ATOM	2754	CA	VAL	A	339	38.270	22.857	14.783	1.00	12.66	6
ATOM	2755	CB	VAL	A	339	36.803	22.594	15.154	1.00	11.55	6
ATOM	2756	CG1	VAL	A	339	36.030	21.874	14.057	1.00	9.87	6

ATOM	2757	CG2	VAL	A	339	36.745	21.811	16.483	1.00	9.86	6
ATOM	2758	C	VAL	A	339	38.513	23.484	13.385	1.00	12.57	6
ATOM	2759	O	VAL	A	339	38.271	24.688	13.279	1.00	12.26	8
ATOM	2760	N	GLN	A	340	39.016	22.686	12.404	1.00	12.55	7
ATOM	2761	CA	GLN	A	340	39.280	23.302	11.088	1.00	12.55	6
ATOM	2762	CB	GLN	A	340	39.975	22.357	10.097	1.00	11.11	6
ATOM	2763	CG	GLN	A	340	41.372	21.974	10.559	1.00	11.55	6
ATOM	2764	CD	GLN	A	340	42.073	21.105	9.513	1.00	14.34	6
ATOM	2765	OE1	GLN	A	340	41.594	20.802	8.384	1.00	15.11	8
ATOM	2766	NE2	GLN	A	340	43.272	20.743	9.959	1.00	12.61	7
ATOM	2767	C	GLN	A	340	38.009	23.900	10.468	1.00	12.34	6
ATOM	2768	O	GLN	A	340	36.930	23.331	10.565	1.00	12.28	8
ATOM	2769	N	THR	A	341	38.147	25.042	9.779	1.00	12.25	7
ATOM	2770	CA	THR	A	341	37.024	25.755	9.200	1.00	12.38	6
ATOM	2771	CB	THR	A	341	37.514	26.993	8.393	1.00	15.06	6
ATOM	2772	OG1	THR	A	341	38.100	27.874	9.353	1.00	16.92	8
ATOM	2773	CG2	THR	A	341	36.347	27.684	7.716	1.00	14.77	6
ATOM	2774	C	THR	A	341	36.124	24.916	8.332	1.00	12.08	6
ATOM	2775	O	THR	A	341	34.910	25.018	8.411	1.00	12.16	8
ATOM	2776	N	TRP	A	342	36.698	24.095	7.465	1.00	11.85	7
ATOM	2777	CA	TRP	A	342	35.902	23.225	6.585	1.00	11.19	6
ATOM	2778	CB	TRP	A	342	36.871	22.438	5.673	1.00	10.89	6
ATOM	2779	CG	TRP	A	342	37.568	21.288	6.392	1.00	9.86	6
ATOM	2780	CD2	TRP	A	342	37.073	19.949	6.491	1.00	9.37	6
ATOM	2781	CE2	TRP	A	342	37.988	19.219	7.276	1.00	9.97	6
ATOM	2782	CE3	TRP	A	342	35.916	19.290	5.991	1.00	10.12	6
ATOM	2783	CD1	TRP	A	342	38.756	21.330	7.062	1.00	10.06	6
ATOM	2784	NE1	TRP	A	342	39.027	20.080	7.592	1.00	11.11	7
ATOM	2785	CZ2	TRP	A	342	37.809	17.853	7.527	1.00	10.50	6
ATOM	2786	CZ3	TRP	A	342	35.700	17.950	6.293	1.00	9.23	6
ATOM	2787	CH2	TRP	A	342	36.654	17.222	7.050	1.00	10.34	6
ATOM	2788	C	TRP	A	342	34.968	22.340	7.391	1.00	10.76	6
ATOM	2789	O	TRP	A	342	33.837	22.038	6.990	1.00	10.60	8
ATOM	2790	N	PHE	A	343	35.375	21.846	8.577	1.00	10.45	7
ATOM	2791	CA	PHE	A	343	34.544	20.979	9.389	1.00	9.81	6
ATOM	2792	CB	PHE	A	343	35.520	20.088	10.193	1.00	10.59	6
ATOM	2793	CG	PHE	A	343	34.841	18.880	10.796	1.00	9.94	6
ATOM	2794	CD1	PHE	A	343	34.561	17.786	9.989	1.00	9.97	6
ATOM	2795	CD2	PHE	A	343	34.466	18.875	12.117	1.00	9.30	6
ATOM	2796	CE1	PHE	A	343	33.947	16.653	10.504	1.00	9.66	6
ATOM	2797	CE2	PHE	A	343	33.842	17.747	12.659	1.00	10.16	6
ATOM	2798	CZ	PHE	A	343	33.592	16.637	11.845	1.00	10.55	6
ATOM	2799	C	PHE	A	343	33.621	21.720	10.332	1.00	9.65	6
ATOM	2800	O	PHE	A	343	32.649	21.140	10.826	1.00	9.50	8
ATOM	2801	N	LYS	A	344	33.897	23.010	10.569	1.00	9.52	7
ATOM	2802	CA	LYS	A	344	33.084	23.775	11.536	1.00	9.73	6
ATOM	2803	CB	LYS	A	344	33.689	25.209	11.614	1.00	11.03	6
ATOM	2804	CG	LYS	A	344	33.193	25.978	12.846	1.00	11.47	6
ATOM	2805	CD	LYS	A	344	34.235	26.954	13.366	1.00	10.60	6
ATOM	2806	CE	LYS	A	344	35.068	26.281	14.470	1.00	9.19	6
ATOM	2807	NZ	LYS	A	344	36.098	27.262	14.962	1.00	7.52	7
ATOM	2808	C	LYS	A	344	31.573	23.696	11.384	1.00	9.62	6
ATOM	2809	O	LYS	A	344	30.838	23.428	12.371	1.00	9.63	8
ATOM	2810	N	PRO	A	345	30.989	23.886	10.213	1.00	9.37	7
ATOM	2811	CD	PRO	A	345	31.697	24.236	8.991	1.00	9.33	6
ATOM	2812	CA	PRO	A	345	29.559	23.779	10.018	1.00	9.01	6
ATOM	2813	CB	PRO	A	345	29.285	24.245	8.592	1.00	9.17	6
ATOM	2814	CG	PRO	A	345	30.576	25.000	8.288	1.00	9.42	6
ATOM	2815	C	PRO	A	345	29.077	22.331	10.309	1.00	8.68	6
ATOM	2816	O	PRO	A	345	27.992	22.162	10.862	1.00	8.28	8
ATOM	2817	N	LEU	A	346	29.863	21.274	9.998	1.00	8.29	7
ATOM	2818	CA	LEU	A	346	29.491	19.890	10.274	1.00	7.82	6
ATOM	2819	CB	LEU	A	346	30.443	18.876	9.664	1.00	7.71	6
ATOM	2820	CG	LEU	A	346	30.608	18.730	8.147	1.00	9.48	6
ATOM	2821	CD1	LEU	A	346	30.910	20.053	7.472	1.00	6.38	6
ATOM	2822	CD2	LEU	A	346	31.710	17.710	7.794	1.00	9.58	6
ATOM	2823	C	LEU	A	346	29.426	19.714	11.796	1.00	7.55	6
ATOM	2824	O	LEU	A	346	28.510	19.084	12.262	1.00	7.43	8
ATOM	2825	N	ALA	A	347	30.320	20.297	12.583	1.00	7.30	7
ATOM	2826	CA	ALA	A	347	30.425	20.274	14.019	1.00	7.11	6
ATOM	2827	CB	ALA	A	347	31.740	20.902	14.501	1.00	7.21	6
ATOM	2828	C	ALA	A	347	29.264	21.031	14.671	1.00	7.06	6
ATOM	2829	O	ALA	A	347	28.712	20.558	15.670	1.00	7.03	8
ATOM	2830	N	TYR	A	348	28.827	22.160	14.103	1.00	7.17	7
ATOM	2831	CA	TYR	A	348	27.673	22.854	14.693	1.00	7.17	6
ATOM	2832	CB	TYR	A	348	27.650	24.299	14.175	1.00	7.45	6
ATOM	2833	CG	TYR	A	348	28.510	25.236	15.008	1.00	7.77	6
ATOM	2834	CD1	TYR	A	348	29.718	25.772	14.609	1.00	7.85	6
ATOM	2835	CE1	TYR	A	348	30.416	26.670	15.415	1.00	7.87	6
ATOM	2836	CD2	TYR	A	348	28.035	25.569	16.285	1.00	7.82	6
ATOM	2837	CE2	TYR	A	348	28.731	26.430	17.105	1.00	7.89	6
ATOM	2838	CZ	TYR	A	348	29.917	26.984	16.682	1.00	7.94	6
ATOM	2839	OH	TYR	A	348	30.609	27.789	17.576	1.00	7.87	8
ATOM	2840	C	TYR	A	348	26.404	22.081	14.387	1.00	7.12	6
ATOM	2841	O	TYR	A	348	25.461	22.029	15.193	1.00	7.05	8
ATOM	2842	N	ALA	A	349	26.328	21.385	13.223	1.00	6.87	7
ATOM	2843	CA	ALA	A	349	25.127	20.607	12.939	1.00	6.67	6
ATOM	2844	CB	ALA	A	349	25.131	20.070	11.515	1.00	6.51	6
ATOM	2845	C	ALA	A	349	25.054	19.497	13.978	1.00	6.62	6
ATOM	2846	O	ALA	A	349	23.995	19.114	14.487	1.00	6.43	8
ATOM	2847	N	PHE	A	350	26.237	18.899	14.250	1.00	6.67	7
ATOM	2848	CA	PHE	A	350	26.268	17.814	15.220	1.00	6.81	6
ATOM	2849	CB	PHE	A	350	27.701	17.250	15.304	1.00	6.91	6
ATOM	2850	CG	PHE	A	350	27.746	15.996	16.137	1.00	9.15	6
ATOM	2851	CD1	PHE	A	350	27.494	14.763	15.559	1.00	8.95	6
ATOM	2852	CD2	PHE	A	350	28.009	16.069	17.510	1.00	11.23	6
ATOM	2853	CE1	PHE	A	350	27.551	13.618	16.317	1.00	10.89	6
ATOM	2854	CE2	PHE	A	350	28.044	14.894	18.273	1.00	11.66	6
ATOM	2855	CZ	PHE	A	350	27.847	13.657	17.687	1.00	10.74	6
ATOM	2856	C	PHE	A	350	25.768	18.242	16.605	1.00	6.90	6
ATOM	2857	O	PHE	A	350	24.978	17.547	17.275	1.00	6.86	8
ATOM	2858	N	ILE	A	351	26.217	19.408	17.102	1.00	7.14	7
ATOM	2859	CA	ILE	A	351	25.736	19.797	18.437	1.00	7.28	6
ATOM	2860	CB	ILE	A	351	26.767	20.663	19.194	1.00	6.43	6
ATOM	2861	CG2	ILE	A	351	28.084	19.924	19.275	1.00	6.52	6
ATOM	2862	CG1	ILE	A	351	26.943	22.024	18.556	1.00	6.43	6

ATOM	2863	CD1	ILE	A	351	27.589	22.986	19.575	1.00	5.33	6
ATOM	2864	C	ILE	A	351	24.372	20.509	18.459	1.00	7.26	6
ATOM	2865	O	ILE	A	351	23.668	20.349	19.498	1.00	7.46	8
ATOM	2866	N	LEU	A	352	23.960	21.213	17.423	1.00	7.13	7
ATOM	2867	CA	LEU	A	352	22.678	21.931	17.500	1.00	7.51	6
ATOM	2868	CB	LEU	A	352	22.778	23.170	16.614	1.00	6.11	6
ATOM	2869	CG	LEU	A	352	23.789	24.248	17.000	1.00	7.70	6
ATOM	2870	CD1	LEU	A	352	23.973	25.292	15.878	1.00	6.26	6
ATOM	2871	CD2	LEU	A	352	23.307	24.932	18.273	1.00	6.10	6
ATOM	2872	C	LEU	A	352	21.377	21.209	17.097	1.00	7.69	6
ATOM	2873	O	LEU	A	352	20.314	21.664	17.512	1.00	7.18	8
ATOM	2874	N	THR	A	353	21.530	20.143	16.291	1.00	8.22	7
ATOM	2875	CA	THR	A	353	20.394	19.372	15.781	1.00	9.02	6
ATOM	2876	CB	THR	A	353	20.420	19.145	14.234	1.00	9.08	6
ATOM	2877	OG1	THR	A	353	21.434	18.262	13.784	1.00	8.55	8
ATOM	2878	CG2	THR	A	353	20.559	20.504	13.545	1.00	9.72	6
ATOM	2879	C	THR	A	353	20.161	18.030	16.481	1.00	9.71	6
ATOM	2880	O	THR	A	353	19.066	17.453	16.250	1.00	9.88	8
ATOM	2881	N	ARG	A	354	21.086	17.601	17.369	1.00	10.05	7
ATOM	2882	CA	ARG	A	354	20.883	16.330	18.085	1.00	10.58	6
ATOM	2883	CB	ARG	A	354	22.258	15.688	18.208	1.00	9.90	6
ATOM	2884	CG	ARG	A	354	22.706	15.117	16.879	1.00	8.76	6
ATOM	2885	CD	ARG	A	354	24.107	14.517	17.011	1.00	9.60	6
ATOM	2886	NE	ARG	A	354	24.016	13.348	17.864	1.00	8.67	7
ATOM	2887	CZ	ARG	A	354	23.434	12.222	17.541	1.00	9.03	6
ATOM	2888	NH1	ARG	A	354	23.392	11.309	18.513	1.00	10.30	7
ATOM	2889	NH2	ARG	A	354	22.866	11.890	16.408	1.00	8.32	7
ATOM	2890	C	ARG	A	354	20.103	16.563	19.378	1.00	11.10	6
ATOM	2891	O	ARG	A	354	20.157	17.713	19.854	1.00	11.27	8
ATOM	2892	N	GLU	A	355	19.325	15.618	19.921	1.00	11.22	7
ATOM	2893	CA	GLU	A	355	18.560	15.818	21.130	1.00	11.61	6
ATOM	2894	CB	GLU	A	355	17.527	14.661	21.351	1.00	14.92	6
ATOM	2895	CG	GLU	A	355	18.229	13.320	21.567	1.00	17.30	6
ATOM	2896	CD	GLU	A	355	17.370	12.087	21.646	1.00	19.96	6
ATOM	2897	OE1	GLU	A	355	17.828	10.936	21.901	1.00	21.87	8
ATOM	2898	OE2	GLU	A	355	16.145	12.138	21.394	1.00	22.12	8
ATOM	2899	C	GLU	A	355	19.317	15.898	22.469	1.00	11.55	6
ATOM	2900	O	GLU	A	355	18.718	16.405	23.441	1.00	11.55	8
ATOM	2901	N	SER	A	356	20.569	15.450	22.576	1.00	11.30	7
ATOM	2902	CA	SER	A	356	21.130	15.577	23.939	1.00	11.56	6
ATOM	2903	CB	SER	A	356	21.398	14.171	24.475	1.00	13.81	6
ATOM	2904	OG	SER	A	356	22.246	13.514	23.552	1.00	18.62	8
ATOM	2905	C	SER	A	356	22.241	16.607	23.975	1.00	11.33	6
ATOM	2906	O	SER	A	356	22.863	16.940	22.971	1.00	11.70	8
ATOM	2907	N	GLY	A	357	22.426	17.219	25.136	1.00	10.87	7
ATOM	2908	CA	GLY	A	357	23.363	18.269	25.422	1.00	10.39	6
ATOM	2909	C	GLY	A	357	22.619	19.622	25.239	1.00	10.36	6
ATOM	2910	O	GLY	A	357	21.602	19.837	24.547	1.00	10.17	8
ATOM	2911	N	TYR	A	358	23.255	20.608	25.880	1.00	10.01	7
ATOM	2912	CA	TYR	A	358	22.884	22.017	25.877	1.00	9.76	6
ATOM	2913	CB	TYR	A	358	22.669	22.498	27.311	1.00	9.60	6
ATOM	2914	CG	TYR	A	358	22.268	23.937	27.516	1.00	9.61	6
ATOM	2915	CD1	TYR	A	358	21.829	24.775	26.494	1.00	9.48	6
ATOM	2916	CE1	TYR	A	358	21.449	26.080	26.747	1.00	9.42	6
ATOM	2917	CD2	TYR	A	358	22.294	24.466	28.799	1.00	9.67	6
ATOM	2918	CE2	TYR	A	358	21.900	25.783	29.085	1.00	9.55	6
ATOM	2919	CZ	TYR	A	358	21.466	26.587	28.050	1.00	9.41	6
ATOM	2920	OH	TYR	A	358	21.076	27.879	28.304	1.00	8.90	8
ATOM	2921	C	TYR	A	358	24.062	22.642	25.113	1.00	9.49	6
ATOM	2922	O	TYR	A	358	25.195	22.737	25.552	1.00	9.20	8
ATOM	2923	N	PRO	A	359	23.809	22.981	23.858	1.00	9.59	7
ATOM	2924	CD	PRO	A	359	22.503	22.784	23.206	1.00	9.74	6
ATOM	2925	CA	PRO	A	359	24.786	23.481	22.907	1.00	9.51	6
ATOM	2926	CB	PRO	A	359	24.249	23.201	21.495	1.00	9.51	6
ATOM	2927	CG	PRO	A	359	22.763	23.211	21.778	1.00	9.71	6
ATOM	2928	C	PRO	A	359	25.173	24.945	23.045	1.00	9.55	6
ATOM	2929	O	PRO	A	359	24.319	25.756	23.334	1.00	9.40	8
ATOM	2930	N	GLN	A	360	26.454	25.242	22.837	1.00	9.58	7
ATOM	2931	CA	GLN	A	360	26.970	26.588	22.963	1.00	9.76	6
ATOM	2932	CB	GLN	A	360	28.115	26.660	24.024	1.00	11.01	6
ATOM	2933	CG	GLN	A	360	28.777	28.065	24.057	1.00	13.99	6
ATOM	2934	CD	GLN	A	360	30.282	28.033	24.332	1.00	15.99	6
ATOM	2935	OE1	GLN	A	360	30.427	27.709	25.524	1.00	14.42	8
ATOM	2936	NE2	GLN	A	360	31.291	28.336	23.425	1.00	15.78	7
ATOM	2937	C	GLN	A	360	27.481	27.096	21.610	1.00	9.39	6
ATOM	2938	O	GLN	A	360	28.228	26.305	21.007	1.00	9.32	8
ATOM	2939	N	VAL	A	361	27.111	28.317	21.278	1.00	9.24	7
ATOM	2940	CA	VAL	A	361	27.586	28.925	20.022	1.00	9.26	6
ATOM	2941	CB	VAL	A	361	26.532	29.709	19.230	1.00	10.17	6
ATOM	2942	CG1	VAL	A	361	27.159	30.437	18.039	1.00	9.02	6
ATOM	2943	CG2	VAL	A	361	25.394	28.761	18.785	1.00	9.34	6
ATOM	2944	C	VAL	A	361	28.739	29.880	20.354	1.00	9.12	6
ATOM	2945	O	VAL	A	361	28.526	30.595	21.350	1.00	9.34	8
ATOM	2946	N	PHE	A	362	29.879	29.887	19.703	1.00	8.60	7
ATOM	2947	CA	PHE	A	362	30.985	30.768	20.056	1.00	8.23	6
ATOM	2948	CB	PHE	A	362	32.308	30.060	19.804	1.00	5.00	6
ATOM	2949	CG	PHE	A	362	33.606	30.771	20.058	1.00	6.40	6
ATOM	2950	CD1	PHE	A	362	33.778	31.642	21.142	1.00	5.78	6
ATOM	2951	CD2	PHE	A	362	34.710	30.563	19.197	1.00	5.00	6
ATOM	2952	CE1	PHE	A	362	34.961	32.330	21.423	1.00	5.15	6
ATOM	2953	CE2	PHE	A	362	35.912	31.220	19.464	1.00	5.23	6
ATOM	2954	CZ	PHE	A	362	36.039	32.080	20.579	1.00	5.49	6
ATOM	2955	C	PHE	A	362	30.967	32.053	19.251	1.00	8.28	6
ATOM	2956	O	PHE	A	362	30.857	32.004	18.043	1.00	7.85	8
ATOM	2957	N	TYR	A	363	31.117	33.210	19.872	1.00	8.47	7
ATOM	2958	CA	TYR	A	363	31.144	34.545	19.289	1.00	8.84	6
ATOM	2959	CB	TYR	A	363	31.363	35.652	20.344	1.00	9.13	6
ATOM	2960	CG	TYR	A	363	31.530	37.091	19.976	1.00	9.86	6
ATOM	2961	CD1	TYR	A	363	30.479	37.981	20.213	1.00	10.09	6
ATOM	2962	CE1	TYR	A	363	30.585	39.317	19.904	1.00	10.35	6
ATOM	2963	CD2	TYR	A	363	32.709	37.609	19.410	1.00	10.25	6
ATOM	2964	CE2	TYR	A	363	32.850	38.956	19.091	1.00	10.30	6
ATOM	2965	CZ	TYR	A	363	31.776	39.774	19.365	1.00	10.78	6
ATOM	2966	OH	TYR	A	363	31.831	41.126	19.087	1.00	11.58	8
ATOM	2967	C	TYR	A	363	32.241	34.680	18.187	1.00	8.73	6
ATOM	2968	O	TYR	A	363	32.011	35.363	17.191	1.00	8.42	8

SUBSTITUTE SHEET (RULE 26)

Appendix 1

ATOM	2969	N	GLY	A	364	33.399	34.040	18.452	1.00	8.56	7
ATOM	2970	CA	GLY	A	364	34.472	34.061	17.503	1.00	8.81	6
ATOM	2971	C	GLY	A	364	34.083	33.261	16.231	1.00	9.04	6
ATOM	2972	O	GLY	A	364	34.596	33.639	15.156	1.00	8.91	8
ATOM	2973	N	ASP	A	365	33.233	32.251	16.327	1.00	9.21	7
ATOM	2974	CA	ASP	A	365	32.830	31.513	15.137	1.00	9.93	6
ATOM	2975	CB	ASP	A	365	32.255	30.146	15.429	1.00	8.93	6
ATOM	2976	CG	ASP	A	365	33.349	29.235	15.977	1.00	9.58	6
ATOM	2977	OD1	ASP	A	365	34.516	29.422	15.641	1.00	10.56	8
ATOM	2978	OD2	ASP	A	365	33.078	28.275	16.700	1.00	9.75	8
ATOM	2979	C	ASP	A	365	31.780	32.264	14.321	1.00	10.69	6
ATOM	2980	O	ASP	A	365	31.770	32.135	13.078	1.00	10.75	8
ATOM	2981	N	MET	A	366	30.887	32.996	14.980	1.00	11.30	7
ATOM	2982	CA	MET	A	366	29.857	33.792	14.295	1.00	11.93	6
ATOM	2983	CB	MET	A	366	28.838	34.351	15.303	1.00	14.14	6
ATOM	2984	CG	MET	A	366	27.828	33.348	15.827	1.00	17.97	6
ATOM	2985	SD	MET	A	366	26.475	33.032	14.646	1.00	22.02	16
ATOM	2986	CE	MET	A	366	25.576	34.590	14.752	1.00	20.61	6
ATOM	2987	C	MET	A	366	30.455	35.016	13.604	1.00	12.33	6
ATOM	2988	O	MET	A	366	30.240	35.367	12.445	1.00	12.31	8
ATOM	2989	N	TYR	A	367	31.249	35.740	14.417	1.00	12.74	7
ATOM	2990	CA	TYR	A	367	31.831	36.964	13.927	1.00	13.46	6
ATOM	2991	CB	TYR	A	367	31.548	38.065	14.988	1.00	14.31	6
ATOM	2992	CG	TYR	A	367	30.092	38.282	15.374	1.00	15.58	6
ATOM	2993	CD1	TYR	A	367	29.721	38.284	16.730	1.00	15.98	6
ATOM	2994	CE1	TYR	A	367	28.410	38.438	17.141	1.00	16.47	6
ATOM	2995	CD2	TYR	A	367	29.075	38.425	14.433	1.00	16.06	6
ATOM	2996	CE2	TYR	A	367	27.776	38.629	14.845	1.00	16.69	6
ATOM	2997	CZ	TYR	A	367	27.431	38.644	16.196	1.00	16.89	6
ATOM	2998	OH	TYR	A	367	26.105	38.815	16.553	1.00	16.92	8
ATOM	2999	C	TYR	A	367	33.299	36.913	13.589	1.00	13.51	6
ATOM	3000	O	TYR	A	367	33.733	38.005	13.190	1.00	13.49	8
ATOM	3001	N	GLY	A	368	34.050	35.837	13.717	1.00	13.66	7
ATOM	3002	CA	GLY	A	368	35.472	35.957	13.368	1.00	14.18	6
ATOM	3003	C	GLY	A	368	36.289	36.369	14.599	1.00	14.83	6
ATOM	3004	O	GLY	A	368	35.746	36.992	15.528	1.00	15.20	8
ATOM	3005	N	THR	A	369	37.531	35.971	14.691	1.00	14.98	7
ATOM	3006	CA	THR	A	369	38.409	36.330	15.759	1.00	15.75	6
ATOM	3007	CB	THR	A	369	39.185	35.126	16.318	1.00	14.06	6
ATOM	3008	OG1	THR	A	369	39.926	34.392	15.324	1.00	11.76	8
ATOM	3009	CG2	THR	A	369	38.175	34.186	16.966	1.00	10.90	6
ATOM	3010	C	THR	A	369	39.346	37.437	15.225	1.00	16.84	6
ATOM	3011	O	THR	A	369	39.727	37.463	14.039	1.00	16.53	8
ATOM	3012	N	LYS	A	370	39.733	38.369	16.120	1.00	17.86	7
ATOM	3013	CA	LYS	A	370	40.568	39.488	15.712	1.00	19.14	6
ATOM	3014	CB	LYS	A	370	39.849	40.792	16.133	1.00	22.20	6
ATOM	3015	CG	LYS	A	370	38.702	41.073	15.133	1.00	26.42	6
ATOM	3016	CD	LYS	A	370	39.254	41.271	13.736	1.00	29.66	6
ATOM	3017	CE	LYS	A	370	38.326	41.239	12.544	1.00	32.10	6
ATOM	3018	NZ	LYS	A	370	39.111	41.178	11.243	1.00	33.93	7
ATOM	3019	C	LYS	A	370	41.998	39.442	16.214	1.00	19.90	6
ATOM	3020	O	LYS	A	370	42.638	40.436	16.526	1.00	19.78	8
ATOM	3021	N	GLY	A	371	42.534	38.244	16.329	1.00	20.85	7
ATOM	3022	CA	GLY	A	371	43.889	37.991	16.742	1.00	22.15	6
ATOM	3023	C	GLY	A	371	44.817	38.443	15.581	1.00	23.36	6
ATOM	3024	O	GLY	A	371	44.393	38.896	14.521	1.00	23.05	8
ATOM	3025	N	ASP	A	372	46.095	38.223	15.877	1.00	24.83	7
ATOM	3026	CA	ASP	A	372	47.186	38.626	15.016	1.00	26.55	6
ATOM	3027	CB	ASP	A	372	48.323	39.306	15.874	1.00	31.39	6
ATOM	3028	CG	ASP	A	372	47.962	40.791	15.968	1.00	34.93	6
ATOM	3029	OD1	ASP	A	372	47.609	41.363	14.906	1.00	37.36	8
ATOM	3030	OD2	ASP	A	372	47.972	41.443	17.034	1.00	37.47	8
ATOM	3031	C	ASP	A	372	47.796	37.520	14.189	1.00	27.31	6
ATOM	3032	O	ASP	A	372	48.870	37.818	13.613	1.00	27.65	8
ATOM	3033	N	SER	A	373	47.162	36.353	14.146	1.00	27.64	7
ATOM	3034	CA	SER	A	373	47.800	35.318	13.305	1.00	27.95	6
ATOM	3035	CB	SER	A	373	47.678	33.936	13.932	1.00	26.91	6
ATOM	3036	OG	SER	A	373	46.393	33.416	13.642	1.00	28.21	8
ATOM	3037	C	SER	A	373	47.255	35.373	11.873	1.00	28.20	6
ATOM	3038	O	SER	A	373	46.480	36.189	11.366	1.00	28.10	8
ATOM	3039	N	GLN	A	374	47.780	34.393	11.137	1.00	28.61	7
ATOM	3040	CA	GLN	A	374	47.348	34.201	9.729	1.00	28.86	6
ATOM	3041	CB	GLN	A	374	48.525	34.112	8.767	1.00	34.24	6
ATOM	3042	CG	GLN	A	374	49.400	35.309	8.530	1.00	40.44	6
ATOM	3043	CD	GLN	A	374	48.939	36.714	8.874	1.00	45.21	6
ATOM	3044	OE1	GLN	A	374	48.111	37.342	8.149	1.00	47.86	8
ATOM	3045	NE2	GLN	A	374	49.449	37.277	10.005	1.00	45.97	7
ATOM	3046	C	GLN	A	374	46.414	32.963	9.719	1.00	28.21	6
ATOM	3047	O	GLN	A	374	46.105	32.340	8.674	1.00	28.76	8
ATOM	3048	N	ARG	A	375	45.952	32.517	10.873	1.00	26.96	7
ATOM	3049	CA	ARG	A	375	45.066	31.421	11.109	1.00	25.60	6
ATOM	3050	CB	ARG	A	375	45.641	30.394	12.115	1.00	29.84	6
ATOM	3051	CG	ARG	A	375	46.842	29.713	11.509	1.00	33.75	6
ATOM	3052	CD	ARG	A	375	48.088	30.386	12.067	1.00	36.33	6
ATOM	3053	NE	ARG	A	375	48.286	30.141	13.475	1.00	37.64	7
ATOM	3054	CZ	ARG	A	375	47.856	29.261	14.351	1.00	37.09	6
ATOM	3055	NH1	ARG	A	375	47.016	28.308	13.998	1.00	37.77	7
ATOM	3056	NH2	ARG	A	375	48.293	29.399	15.587	1.00	36.83	7
ATOM	3057	C	ARG	A	375	43.777	31.845	11.827	1.00	23.88	6
ATOM	3058	O	ARG	A	375	43.218	30.942	12.450	1.00	23.81	8
ATOM	3059	N	GLU	A	376	43.399	33.116	11.777	1.00	22.28	7
ATOM	3060	CA	GLU	A	376	42.196	33.558	12.450	1.00	20.37	6
ATOM	3061	CB	GLU	A	376	42.061	35.080	12.418	1.00	17.56	6
ATOM	3062	CG	GLU	A	376	43.203	35.780	13.151	1.00	16.13	6
ATOM	3063	CD	GLU	A	376	43.361	35.421	14.595	1.00	14.90	6
ATOM	3064	OE1	GLU	A	376	42.403	35.436	15.391	1.00	12.95	8
ATOM	3065	OE2	GLU	A	376	44.510	35.188	15.051	1.00	16.10	8
ATOM	3066	C	GLU	A	376	40.955	32.886	11.869	1.00	19.17	6
ATOM	3067	O	GLU	A	376	40.801	32.503	10.715	1.00	18.94	8
ATOM	3068	N	ILE	A	377	40.002	32.698	12.777	1.00	18.23	7
ATOM	3069	CA	ILE	A	377	38.726	32.102	12.410	1.00	17.23	6
ATOM	3070	CB	ILE	A	377	37.924	31.634	13.636	1.00	15.28	6
ATOM	3071	CG2	ILE	A	377	36.616	30.961	13.205	1.00	15.23	6
ATOM	3072	CG1	ILE	A	377	38.720	30.715	14.564	1.00	14.23	6
ATOM	3073	CD1	ILE	A	377	38.109	30.512	15.935	1.00	13.53	6
ATOM	3074	C	ILE	A	377	37.957	33.184	11.660	1.00	16.78	6

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ATOM	3075	O	ILE	A	377	37.783	34.301	12.173	1.00	16.90	8
ATOM	3076	N	PRO	A	378	37.461	32.927	10.461	1.00	16.21	7
ATOM	3077	CD	PRO	A	378	37.634	31.617	9.821	1.00	16.04	6
ATOM	3078	CA	PRO	A	378	36.637	33.810	9.695	1.00	15.87	6
ATOM	3079	CB	PRO	A	378	36.555	33.232	8.263	1.00	15.98	6
ATOM	3080	CG	PRO	A	378	37.023	31.835	8.456	1.00	15.94	6
ATOM	3081	C	PRO	A	378	35.214	33.860	10.247	1.00	15.56	6
ATOM	3082	O	PRO	A	378	34.741	32.945	10.946	1.00	15.55	8
ATOM	3083	N	ALA	A	379	34.506	34.960	9.931	1.00	15.19	7
ATOM	3084	CA	ALA	A	379	33.095	35.063	10.370	1.00	14.83	6
ATOM	3085	CB	ALA	A	379	32.523	36.450	10.119	1.00	13.37	6
ATOM	3086	C	ALA	A	379	32.246	33.979	9.679	1.00	14.60	6
ATOM	3087	O	ALA	A	379	32.082	33.990	8.438	1.00	14.65	8
ATOM	3088	N	LEU	A	380	31.703	33.021	10.428	1.00	14.28	7
ATOM	3089	CA	LEU	A	380	30.925	31.960	9.792	1.00	14.14	6
ATOM	3090	CB	LEU	A	380	31.468	30.617	10.265	1.00	15.00	6
ATOM	3091	CG	LEU	A	380	32.913	30.303	9.865	1.00	16.56	6
ATOM	3092	CD1	LEU	A	380	33.486	29.165	10.688	1.00	16.26	6
ATOM	3093	CD2	LEU	A	380	32.975	30.004	8.350	1.00	16.68	6
ATOM	3094	C	LEU	A	380	29.448	32.123	10.017	1.00	14.34	6
ATOM	3095	O	LEU	A	380	28.602	31.262	9.773	1.00	14.38	8
ATOM	3096	N	LYS	A	381	29.011	33.278	10.475	1.00	14.36	7
ATOM	3097	CA	LYS	A	381	27.615	33.579	10.719	1.00	14.84	6
ATOM	3098	CB	LYS	A	381	27.672	35.101	10.820	1.00	18.02	6
ATOM	3099	CG	LYS	A	381	26.382	35.855	10.702	1.00	21.47	6
ATOM	3100	CD	LYS	A	381	26.754	37.314	10.944	1.00	25.20	6
ATOM	3101	CE	LYS	A	381	25.912	38.275	10.104	1.00	28.81	6
ATOM	3102	NZ	LYS	A	381	24.564	38.411	10.770	1.00	30.73	7
ATOM	3103	C	LYS	A	381	26.667	33.106	9.634	1.00	14.98	6
ATOM	3104	O	LYS	A	381	25.589	32.577	9.911	1.00	14.84	8
ATOM	3105	N	HIS	A	382	26.978	33.273	8.350	1.00	14.98	7
ATOM	3106	CA	HIS	A	382	26.079	32.889	7.268	1.00	15.22	6
ATOM	3107	CB	HIS	A	382	26.562	33.593	5.986	1.00	21.24	6
ATOM	3108	CG	HIS	A	382	28.036	33.424	5.842	1.00	25.72	6
ATOM	3109	CD2	HIS	A	382	29.070	33.878	6.615	1.00	27.36	6
ATOM	3110	ND1	HIS	A	382	28.569	32.671	4.810	1.00	28.03	7
ATOM	3111	CE1	HIS	A	382	29.903	32.712	4.939	1.00	28.96	6
ATOM	3112	NE2	HIS	A	382	30.216	33.424	6.041	1.00	28.60	7
ATOM	3113	C	HIS	A	382	25.947	31.415	7.118	1.00	15.05	6
ATOM	3114	O	HIS	A	382	24.948	30.932	6.602	1.00	15.08	8
ATOM	3115	N	LYS	A	383	26.887	30.595	7.622	1.00	14.81	7
ATOM	3116	CA	LYS	A	383	26.802	29.161	7.615	1.00	14.36	6
ATOM	3117	CB	LYS	A	383	28.186	28.551	7.528	1.00	16.14	6
ATOM	3118	CG	LYS	A	383	29.014	29.281	6.505	1.00	20.51	6
ATOM	3119	CD	LYS	A	383	29.147	28.507	5.230	1.00	23.48	6
ATOM	3120	CE	LYS	A	383	30.673	28.350	4.977	1.00	26.30	6
ATOM	3121	NZ	LYS	A	383	31.046	29.207	3.792	1.00	27.91	7
ATOM	3122	C	LYS	A	383	26.207	28.595	8.926	1.00	13.88	6
ATOM	3123	O	LYS	A	383	25.694	27.478	8.956	1.00	13.80	8
ATOM	3124	N	ILE	A	384	26.351	29.374	10.004	1.00	13.23	7
ATOM	3125	CA	ILE	A	384	25.814	28.889	11.252	1.00	12.99	6
ATOM	3126	CB	ILE	A	384	26.609	29.381	12.486	1.00	13.25	6
ATOM	3127	CG2	ILE	A	384	25.905	29.000	13.778	1.00	12.19	6
ATOM	3128	CG1	ILE	A	384	28.029	28.790	12.411	1.00	13.70	6
ATOM	3129	CD1	ILE	A	384	28.902	29.649	13.343	1.00	15.12	6
ATOM	3130	C	ILE	A	384	24.335	29.241	11.430	1.00	12.61	6
ATOM	3131	O	ILE	A	384	23.621	28.363	11.931	1.00	12.68	8
ATOM	3132	N	GLU	A	385	23.841	30.401	11.025	1.00	12.22	7
ATOM	3133	CA	GLU	A	385	22.459	30.804	11.178	1.00	12.09	6
ATOM	3134	CB	GLU	A	385	22.249	32.252	10.671	1.00	13.25	6
ATOM	3135	CG	GLU	A	385	23.039	33.148	11.637	1.00	16.06	6
ATOM	3136	CD	GLU	A	385	22.681	34.621	11.531	1.00	18.04	6
ATOM	3137	OE1	GLU	A	385	22.082	35.050	10.531	1.00	18.27	8
ATOM	3138	OE2	GLU	A	385	22.960	35.427	12.453	1.00	18.60	8
ATOM	3139	C	GLU	A	385	21.439	29.867	10.587	1.00	11.96	6
ATOM	3140	O	GLU	A	385	20.439	29.608	11.273	1.00	12.04	8
ATOM	3141	N	PRO	A	386	21.614	29.238	9.436	1.00	11.74	7
ATOM	3142	CD	PRO	A	386	22.735	29.467	8.528	1.00	11.74	6
ATOM	3143	CA	PRO	A	386	20.676	28.265	8.905	1.00	11.52	6
ATOM	3144	CB	PRO	A	386	21.205	27.847	7.516	1.00	11.54	6
ATOM	3145	CG	PRO	A	386	22.167	28.967	7.199	1.00	11.74	6
ATOM	3146	C	PRO	A	386	20.545	27.050	9.826	1.00	11.28	6
ATOM	3147	O	PRO	A	386	19.493	26.419	9.963	1.00	11.21	8
ATOM	3148	N	ILE	A	387	21.617	26.648	10.530	1.00	11.05	7
ATOM	3149	CA	ILE	A	387	21.619	25.492	11.424	1.00	10.84	6
ATOM	3150	CB	ILE	A	387	23.047	24.957	11.653	1.00	8.79	6
ATOM	3151	CG2	ILE	A	387	22.978	23.619	12.340	1.00	6.90	6
ATOM	3152	CG1	ILE	A	387	23.799	24.850	10.310	1.00	8.27	6
ATOM	3153	CD1	ILE	A	387	25.231	24.430	10.511	1.00	9.38	6
ATOM	3154	C	ILE	A	387	20.917	25.808	12.754	1.00	11.01	6
ATOM	3155	O	ILE	A	387	20.273	24.946	13.366	1.00	10.92	8
ATOM	3156	N	LEU	A	388	21.058	27.064	13.176	1.00	11.09	7
ATOM	3157	CA	LEU	A	388	20.400	27.620	14.345	1.00	11.19	6
ATOM	3158	CB	LEU	A	388	20.902	29.010	14.682	1.00	10.46	6
ATOM	3159	CG	LEU	A	388	22.084	29.061	15.638	1.00	11.84	6
ATOM	3160	CD1	LEU	A	388	22.502	30.545	15.745	1.00	11.69	6
ATOM	3161	CD2	LEU	A	388	21.636	28.377	16.916	1.00	10.70	6
ATOM	3162	C	LEU	A	388	18.887	27.688	14.042	1.00	11.21	6
ATOM	3163	O	LEU	A	388	18.017	27.443	14.899	1.00	11.36	8
ATOM	3164	N	LYS	A	389	18.551	28.015	12.792	1.00	11.22	7
ATOM	3165	CA	LYS	A	389	17.142	28.017	12.353	1.00	11.08	6
ATOM	3166	CB	LYS	A	389	17.014	28.553	10.952	1.00	14.65	6
ATOM	3167	CG	LYS	A	389	15.591	28.665	10.402	1.00	20.09	6
ATOM	3168	CD	LYS	A	389	15.454	30.134	9.985	1.00	24.33	6
ATOM	3169	CE	LYS	A	389	14.860	30.232	8.592	1.00	27.30	6
ATOM	3170	NZ	LYS	A	389	13.649	29.337	8.568	1.00	30.42	7
ATOM	3171	C	LYS	A	389	16.620	26.566	12.377	1.00	10.52	6
ATOM	3172	O	LYS	A	389	15.474	26.300	12.746	1.00	10.45	8
ATOM	3173	N	ALA	A	390	17.445	25.613	11.937	1.00	10.03	7
ATOM	3174	CA	ALA	A	390	17.007	24.226	12.020	1.00	9.88	6
ATOM	3175	CB	ALA	A	390	17.970	23.263	11.375	1.00	7.86	6
ATOM	3176	C	ALA	A	390	16.848	23.832	13.506	1.00	9.86	6
ATOM	3177	O	ALA	A	390	15.876	23.103	13.761	1.00	9.92	8
ATOM	3178	N	ARG	A	391	17.713	24.258	14.440	1.00	9.66	7
ATOM	3179	CA	ARG	A	391	17.540	23.914	15.857	1.00	9.64	6
ATOM	3180	CB	ARG	A	391	18.666	24.410	16.800	1.00	8.27	6

SUBSTITUTE SHEET (RULE 26)

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ATOM	3181	CG	ARG	A	391	18.295	24.255	18.295	1.00	6.17	6
ATOM	3182	CD	ARG	A	391	19.637	24.301	19.079	1.00	6.11	6
ATOM	3183	NE	ARG	A	391	19.415	23.982	20.476	1.00	6.39	7
ATOM	3184	CZ	ARG	A	391	19.411	22.752	21.057	1.00	8.41	6
ATOM	3185	NH1	ARG	A	391	19.671	21.719	20.264	1.00	7.01	7
ATOM	3186	NH2	ARG	A	391	19.147	22.533	22.359	1.00	6.75	7
ATOM	3187	C	ARG	A	391	16.258	24.518	16.434	1.00	9.84	6
ATOM	3188	O	ARG	A	391	15.482	23.860	17.089	1.00	9.35	8
ATOM	3189	N	LYS	A	392	16.061	25.811	16.184	1.00	10.42	7
ATOM	3190	CA	LYS	A	392	14.904	26.555	16.666	1.00	11.31	6
ATOM	3191	CB	LYS	A	392	15.137	28.036	16.253	1.00	13.27	6
ATOM	3192	CG	LYS	A	392	14.066	28.928	16.797	1.00	16.07	6
ATOM	3193	CD	LYS	A	392	14.176	30.388	16.369	1.00	20.09	6
ATOM	3194	CE	LYS	A	392	12.806	31.069	16.665	1.00	23.10	6
ATOM	3195	NZ	LYS	A	392	12.989	32.560	16.682	1.00	26.05	7
ATOM	3196	C	LYS	A	392	13.536	26.046	16.200	1.00	11.94	6
ATOM	3197	O	LYS	A	392	12.590	25.903	17.011	1.00	11.92	8
ATOM	3198	N	GLN	A	393	13.349	25.676	14.916	1.00	12.38	7
ATOM	3199	CA	GLN	A	393	12.091	25.218	14.386	1.00	12.80	6
ATOM	3200	CB	GLN	A	393	11.736	25.947	13.069	1.00	17.13	6
ATOM	3201	CG	GLN	A	393	12.463	27.237	12.917	1.00	24.67	6
ATOM	3202	CD	GLN	A	393	11.701	28.402	12.316	1.00	29.33	6
ATOM	3203	OE1	GLN	A	393	11.924	28.717	11.149	1.00	30.64	8
ATOM	3204	NE2	GLN	A	393	10.856	29.003	13.159	1.00	31.70	7
ATOM	3205	C	GLN	A	393	11.921	23.764	13.940	1.00	12.57	6
ATOM	3206	O	GLN	A	393	10.718	23.422	13.839	1.00	12.77	8
ATOM	3207	N	TYR	A	394	12.995	23.041	13.678	1.00	11.99	7
ATOM	3208	CA	TYR	A	394	12.839	21.690	13.167	1.00	11.56	6
ATOM	3209	CB	TYR	A	394	13.577	21.661	11.798	1.00	11.71	6
ATOM	3210	CG	TYR	A	394	12.942	22.687	10.852	1.00	12.27	6
ATOM	3211	CD1	TYR	A	394	13.444	23.941	10.588	1.00	12.30	6
ATOM	3212	CE1	TYR	A	394	12.811	24.826	9.747	1.00	12.61	6
ATOM	3213	CD2	TYR	A	394	11.754	22.328	10.236	1.00	12.73	6
ATOM	3214	CE2	TYR	A	394	11.066	23.192	9.378	1.00	13.02	6
ATOM	3215	CZ	TYR	A	394	11.615	24.442	9.136	1.00	13.05	6
ATOM	3216	OH	TYR	A	394	10.942	25.224	8.229	1.00	13.25	8
ATOM	3217	C	TYR	A	394	13.360	20.552	14.017	1.00	11.27	6
ATOM	3218	O	TYR	A	394	12.866	19.424	13.834	1.00	10.94	8
ATOM	3219	N	ALA	A	395	14.338	20.794	14.908	1.00	10.88	7
ATOM	3220	CA	ALA	A	395	14.896	19.692	15.694	1.00	10.74	6
ATOM	3221	CB	ALA	A	395	16.305	20.151	16.074	1.00	8.72	6
ATOM	3222	C	ALA	A	395	14.101	19.267	16.920	1.00	10.85	6
ATOM	3223	O	ALA	A	395	14.392	19.591	18.082	1.00	10.94	8
ATOM	3224	N	TYR	A	396	12.986	18.545	16.743	1.00	10.85	7
ATOM	3225	CA	TYR	A	396	12.061	18.070	17.753	1.00	10.83	6
ATOM	3226	CB	TYR	A	396	10.763	18.949	17.821	1.00	10.80	6
ATOM	3227	CG	TYR	A	396	11.083	20.390	18.180	1.00	10.52	6
ATOM	3228	CD1	TYR	A	396	11.333	21.365	17.195	1.00	10.49	6
ATOM	3229	CE1	TYR	A	396	11.683	22.665	17.546	1.00	10.23	6
ATOM	3230	CD2	TYR	A	396	11.215	20.744	19.504	1.00	10.24	6
ATOM	3231	CE2	TYR	A	396	11.536	22.043	19.835	1.00	10.18	6
ATOM	3232	CZ	TYR	A	396	11.799	22.984	18.874	1.00	10.23	6
ATOM	3233	OH	TYR	A	396	12.200	24.237	19.305	1.00	10.59	8
ATOM	3234	C	TYR	A	396	11.624	16.631	17.499	1.00	10.90	6
ATOM	3235	O	TYR	A	396	11.615	16.137	16.372	1.00	10.58	8
ATOM	3236	N	GLY	A	397	11.252	15.899	18.555	1.00	11.07	7
ATOM	3237	CA	GLY	A	397	10.772	14.542	18.296	1.00	11.32	6
ATOM	3238	C	GLY	A	397	11.808	13.450	18.353	1.00	11.58	6
ATOM	3239	O	GLY	A	397	13.001	13.761	18.466	1.00	12.00	8
ATOM	3240	N	ALA	A	398	11.341	12.228	18.304	1.00	11.57	7
ATOM	3241	CA	ALA	A	398	12.172	11.044	18.341	1.00	11.80	6
ATOM	3242	CB	ALA	A	398	11.261	9.824	18.105	1.00	9.85	6
ATOM	3243	C	ALA	A	398	13.348	11.115	17.365	1.00	12.04	6
ATOM	3244	O	ALA	A	398	13.259	11.447	16.176	1.00	12.09	8
ATOM	3245	N	GLN	A	399	14.532	10.718	17.833	1.00	12.00	7
ATOM	3246	CA	GLN	A	399	15.761	10.691	17.058	1.00	12.04	6
ATOM	3247	CB	GLN	A	399	16.871	11.357	17.912	1.00	10.48	6
ATOM	3248	CG	GLN	A	399	18.261	11.287	17.346	1.00	9.54	6
ATOM	3249	CD	GLN	A	399	19.195	12.269	18.066	1.00	9.97	6
ATOM	3250	OE1	GLN	A	399	18.983	13.467	18.191	1.00	8.29	8
ATOM	3251	NE2	GLN	A	399	20.306	11.751	18.528	1.00	9.30	7
ATOM	3252	C	GLN	A	399	16.212	9.307	16.643	1.00	12.27	6
ATOM	3253	O	GLN	A	399	16.138	8.327	17.361	1.00	12.29	8
ATOM	3254	N	HIS	A	400	16.765	9.135	15.415	1.00	12.36	7
ATOM	3255	CA	HIS	A	400	17.270	7.893	14.903	1.00	12.28	6
ATOM	3256	CB	HIS	A	400	16.419	7.243	13.800	1.00	12.34	6
ATOM	3257	CG	HIS	A	400	15.001	6.998	14.252	1.00	13.76	6
ATOM	3258	CD2	HIS	A	400	14.464	6.087	15.135	1.00	12.53	6
ATOM	3259	ND1	HIS	A	400	13.959	7.856	13.831	1.00	13.34	7
ATOM	3260	CE1	HIS	A	400	12.860	7.408	14.435	1.00	11.97	6
ATOM	3261	NE2	HIS	A	400	13.095	6.378	15.194	1.00	11.69	7
ATOM	3262	C	HIS	A	400	18.710	8.179	14.411	1.00	12.21	6
ATOM	3263	O	HIS	A	400	18.909	9.132	13.670	1.00	11.78	8
ATOM	3264	N	ASP	A	401	19.651	7.332	14.895	1.00	12.31	7
ATOM	3265	CA	ASP	A	401	21.043	7.503	14.536	1.00	12.71	6
ATOM	3266	CB	ASP	A	401	21.964	7.308	15.758	1.00	15.32	6
ATOM	3267	CG	ASP	A	401	21.883	8.427	16.767	1.00	18.10	6
ATOM	3268	OD1	ASP	A	401	21.438	9.578	16.520	1.00	20.24	8
ATOM	3269	OD2	ASP	A	401	22.299	8.187	17.921	1.00	19.29	8
ATOM	3270	C	ASP	A	401	21.556	6.515	13.484	1.00	12.57	6
ATOM	3271	O	ASP	A	401	21.145	5.360	13.483	1.00	12.31	8
ATOM	3272	N	TYR	A	402	22.385	6.972	12.584	1.00	12.55	7
ATOM	3273	CA	TYR	A	402	22.977	6.173	11.524	1.00	12.83	6
ATOM	3274	CB	TYR	A	402	22.385	6.495	10.130	1.00	12.68	6
ATOM	3275	CG	TYR	A	402	20.891	6.179	10.105	1.00	12.98	6
ATOM	3276	CD1	TYR	A	402	19.990	7.186	10.470	1.00	13.23	6
ATOM	3277	CE1	TYR	A	402	18.631	6.952	10.544	1.00	13.64	6
ATOM	3278	CD2	TYR	A	402	20.378	4.927	9.801	1.00	13.10	6
ATOM	3279	CE2	TYR	A	402	19.018	4.654	9.819	1.00	13.39	6
ATOM	3280	CZ	TYR	A	402	18.168	5.676	10.195	1.00	14.02	6
ATOM	3281	OH	TYR	A	402	16.795	5.502	10.282	1.00	14.72	8
ATOM	3282	C	TYR	A	402	24.478	6.371	11.592	1.00	13.30	6
ATOM	3283	O	TYR	A	402	25.019	7.054	10.747	1.00	13.17	8
ATOM	3284	N	PHE	A	403	25.162	5.818	12.581	1.00	14.08	7
ATOM	3285	CA	PHE	A	403	26.591	5.861	12.792	1.00	14.73	6
ATOM	3286	CB	PHE	A	403	26.978	6.035	14.266	1.00	16.26	6

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ATOM	3287	CG	PHE	A	403	26.766	7.486	14.665	1.00	19.71	6
ATOM	3288	CD1	PHE	A	403	25.574	7.927	15.176	1.00	20.07	6
ATOM	3289	CD2	PHE	A	403	27.748	8.440	14.483	1.00	21.01	6
ATOM	3290	CE1	PHE	A	403	25.379	9.241	15.534	1.00	21.71	6
ATOM	3291	CE2	PHE	A	403	27.540	9.786	14.804	1.00	22.26	6
ATOM	3292	CZ	PHE	A	403	26.338	10.216	15.345	1.00	21.47	6
ATOM	3293	C	PHE	A	403	27.113	4.537	12.220	1.00	15.16	6
ATOM	3294	O	PHE	A	403	27.616	3.625	12.902	1.00	15.23	8
ATOM	3295	N	ASP	A	404	26.987	4.370	10.906	1.00	15.33	7
ATOM	3296	CA	ASP	A	404	27.398	3.103	10.294	1.00	15.59	6
ATOM	3297	CB	ASP	A	404	26.115	2.428	9.754	1.00	17.33	6
ATOM	3298	CG	ASP	A	404	25.433	3.431	8.838	1.00	19.38	6
ATOM	3299	OD1	ASP	A	404	25.870	4.570	8.544	1.00	19.96	8
ATOM	3300	OD2	ASP	A	404	24.330	3.060	8.407	1.00	21.24	8
ATOM	3301	C	ASP	A	404	28.346	3.116	9.119	1.00	15.47	6
ATOM	3302	O	ASP	A	404	28.339	2.154	8.320	1.00	15.71	8
ATOM	3303	N	HIS	A	405	29.168	4.144	8.997	1.00	15.11	7
ATOM	3304	CA	HIS	A	405	30.098	4.238	7.885	1.00	14.80	6
ATOM	3305	CB	HIS	A	405	29.332	4.915	6.719	1.00	14.80	6
ATOM	3306	CG	HIS	A	405	30.187	4.926	5.492	1.00	15.21	6
ATOM	3307	CD2	HIS	A	405	30.385	3.954	4.561	1.00	15.68	6
ATOM	3308	ND1	HIS	A	405	30.992	5.990	5.157	1.00	15.84	7
ATOM	3309	CE1	HIS	A	405	31.654	5.723	4.041	1.00	16.58	6
ATOM	3310	NE2	HIS	A	405	31.309	4.491	3.680	1.00	17.15	7
ATOM	3311	C	HIS	A	405	31.280	5.023	8.383	1.00	14.46	6
ATOM	3312	O	HIS	A	405	31.008	5.908	9.197	1.00	14.63	8
ATOM	3313	N	HIS	A	406	32.494	4.841	7.963	1.00	14.11	7
ATOM	3314	CA	HIS	A	406	33.630	5.587	8.495	1.00	13.78	6
ATOM	3315	CB	HIS	A	406	35.000	4.932	8.189	1.00	15.67	6
ATOM	3316	CG	HIS	A	406	34.981	4.416	6.777	1.00	16.76	6
ATOM	3317	CD2	HIS	A	406	34.450	3.285	6.232	1.00	16.51	6
ATOM	3318	ND1	HIS	A	406	35.504	5.164	5.733	1.00	18.12	7
ATOM	3319	CE1	HIS	A	406	35.318	4.505	4.578	1.00	16.95	6
ATOM	3320	NE2	HIS	A	406	34.666	3.388	4.880	1.00	17.55	7
ATOM	3321	C	HIS	A	406	33.580	7.002	8.026	1.00	13.47	6
ATOM	3322	O	HIS	A	406	34.298	7.753	8.672	1.00	13.10	8
ATOM	3323	N	ASP	A	407	32.861	7.500	7.048	1.00	13.42	7
ATOM	3324	CA	ASP	A	407	32.837	8.877	6.628	1.00	13.27	6
ATOM	3325	CB	ASP	A	407	33.163	9.063	5.138	1.00	14.59	6
ATOM	3326	CG	ASP	A	407	34.556	8.665	4.654	1.00	16.13	6
ATOM	3327	OD1	ASP	A	407	35.474	8.360	5.486	1.00	14.23	8
ATOM	3328	OD2	ASP	A	407	34.808	8.646	3.381	1.00	18.38	8
ATOM	3329	C	ASP	A	407	31.457	9.532	6.757	1.00	12.98	6
ATOM	3330	O	ASP	A	407	31.310	10.601	7.360	1.00	12.77	8
ATOM	3331	N	ILE	A	408	30.465	8.890	6.167	1.00	12.85	7
ATOM	3332	CA	ILE	A	408	29.098	9.438	6.133	1.00	12.79	6
ATOM	3333	CB	ILE	A	408	28.429	9.103	4.799	1.00	14.07	6
ATOM	3334	CG2	ILE	A	408	27.045	9.742	4.656	1.00	12.86	6
ATOM	3335	CG1	ILE	A	408	29.251	9.578	3.597	1.00	13.69	6
ATOM	3336	CD1	ILE	A	408	28.979	8.781	2.321	1.00	14.63	6
ATOM	3337	C	ILE	A	408	28.219	8.885	7.260	1.00	12.60	6
ATOM	3338	O	ILE	A	408	27.838	7.712	7.271	1.00	12.81	8
ATOM	3339	N	VAL	A	409	27.910	9.762	8.195	1.00	12.05	7
ATOM	3340	CA	VAL	A	409	27.012	9.436	9.309	1.00	11.68	6
ATOM	3341	CB	VAL	A	409	27.735	9.616	10.638	1.00	13.02	6
ATOM	3342	CG1	VAL	A	409	28.916	8.661	10.804	1.00	14.14	6
ATOM	3343	CG2	VAL	A	409	28.293	11.030	10.817	1.00	11.59	6
ATOM	3344	C	VAL	A	409	25.823	10.380	9.245	1.00	11.38	6
ATOM	3345	O	VAL	A	409	25.887	11.441	8.613	1.00	11.38	8
ATOM	3346	N	GLY	A	410	24.747	10.000	9.898	1.00	10.96	7
ATOM	3347	CA	GLY	A	410	23.548	10.842	9.910	1.00	10.41	6
ATOM	3348	C	GLY	A	410	22.635	10.508	11.084	1.00	9.89	6
ATOM	3349	O	GLY	A	410	22.871	9.547	11.830	1.00	9.68	8
ATOM	3350	N	TRP	A	411	21.623	11.347	11.201	1.00	9.60	7
ATOM	3351	CA	TRP	A	411	20.569	11.201	12.204	1.00	9.34	6
ATOM	3352	CB	TRP	A	411	20.994	11.750	13.574	1.00	8.12	6
ATOM	3353	CG	TRP	A	411	21.417	13.213	13.561	1.00	8.50	6
ATOM	3354	CD2	TRP	A	411	22.726	13.662	13.285	1.00	8.48	6
ATOM	3355	CE2	TRP	A	411	22.699	15.049	13.356	1.00	8.47	6
ATOM	3356	CE3	TRP	A	411	23.924	13.010	12.971	1.00	9.18	6
ATOM	3357	CD1	TRP	A	411	20.647	14.285	13.808	1.00	6.27	6
ATOM	3358	NE1	TRP	A	411	21.483	15.439	13.671	1.00	6.58	7
ATOM	3359	CZ2	TRP	A	411	23.830	15.839	13.113	1.00	9.15	6
ATOM	3360	CZ3	TRP	A	411	25.054	13.814	12.732	1.00	9.35	6
ATOM	3361	CH2	TRP	A	411	25.007	15.163	12.799	1.00	9.69	6
ATOM	3362	C	TRP	A	411	19.296	11.897	11.708	1.00	9.23	6
ATOM	3363	O	TRP	A	411	19.372	12.824	10.901	1.00	8.76	8
ATOM	3364	N	THR	A	412	18.151	11.418	12.226	1.00	9.36	7
ATOM	3365	CA	THR	A	412	16.877	12.015	11.894	1.00	9.69	6
ATOM	3366	CB	THR	A	412	15.968	11.081	11.040	1.00	10.82	6
ATOM	3367	OG1	THR	A	412	15.687	9.914	11.826	1.00	12.10	8
ATOM	3368	CG2	THR	A	412	16.614	10.613	9.743	1.00	9.28	6
ATOM	3369	C	THR	A	412	16.136	12.441	13.173	1.00	9.93	6
ATOM	3370	O	THR	A	412	16.399	12.027	14.318	1.00	9.78	8
ATOM	3371	N	ARG	A	413	15.184	13.348	12.978	1.00	10.07	7
ATOM	3372	CA	ARG	A	413	14.332	13.843	14.055	1.00	10.74	6
ATOM	3373	CB	ARG	A	413	14.635	15.236	14.615	1.00	8.23	6
ATOM	3374	CG	ARG	A	413	16.039	15.382	15.182	1.00	6.55	6
ATOM	3375	CD	ARG	A	413	16.262	14.604	16.464	1.00	6.58	6
ATOM	3376	NE	ARG	A	413	15.388	14.982	17.577	1.00	5.58	7
ATOM	3377	CZ	ARG	A	413	15.602	16.062	18.326	1.00	8.01	6
ATOM	3378	NH1	ARG	A	413	14.802	16.370	19.349	1.00	7.49	7
ATOM	3379	NH2	ARG	A	413	16.645	16.870	18.094	1.00	7.65	7
ATOM	3380	C	ARG	A	413	12.946	13.767	13.403	1.00	11.41	6
ATOM	3381	O	ARG	A	413	12.678	14.374	12.355	1.00	11.24	8
ATOM	3382	N	GLU	A	414	12.076	12.980	14.035	1.00	12.08	7
ATOM	3383	CA	GLU	A	414	10.713	12.785	13.510	1.00	12.84	6
ATOM	3384	CB	GLU	A	414	9.957	11.626	14.195	1.00	11.98	6
ATOM	3385	CG	GLU	A	414	10.578	10.270	13.880	1.00	12.67	6
ATOM	3386	CD	GLU	A	414	9.722	9.123	14.401	1.00	14.64	6
ATOM	3387	OE1	GLU	A	414	8.485	9.240	14.504	1.00	14.73	8
ATOM	3388	OE2	GLU	A	414	10.249	8.041	14.723	1.00	15.78	8
ATOM	3389	C	GLU	A	414	9.819	14.015	13.605	1.00	13.32	6
ATOM	3390	O	GLU	A	414	8.855	14.006	12.864	1.00	13.17	8
ATOM	3391	N	GLY	A	415	10.096	15.006	14.389	1.00	14.06	7
ATOM	3392	CA	GLY	A	415	9.223	16.150	14.467	1.00	15.71	6

SUBSTITUTE SHEET (RULE 26)

Appendix 1

ATOM	3393	C	GLY	A	415	8.276	15.870	15.637	1.00	17.18	6
ATOM	3394	O	GLY	A	415	8.176	14.768	16.148	1.00	17.23	8
ATOM	3395	N	ASP	A	416	7.581	16.904	16.048	1.00	18.70	7
ATOM	3396	CA	ASP	A	416	6.606	16.860	17.118	1.00	20.18	6
ATOM	3397	CB	ASP	A	416	7.228	17.531	18.307	1.00	26.49	6
ATOM	3398	CG	ASP	A	416	6.358	17.615	19.535	1.00	31.33	6
ATOM	3399	OD1	ASP	A	416	6.791	18.402	20.413	1.00	35.28	8
ATOM	3400	OD2	ASP	A	416	5.301	16.975	19.696	1.00	32.88	8
ATOM	3401	C	ASP	A	416	5.400	17.597	16.568	1.00	21.08	6
ATOM	3402	O	ASP	A	416	5.423	18.631	15.908	1.00	20.94	8
ATOM	3403	N	SER	A	417	4.234	17.031	16.824	1.00	22.16	7
ATOM	3404	CA	SER	A	417	2.928	17.484	16.380	1.00	23.18	6
ATOM	3405	CB	SER	A	417	1.868	16.471	16.846	1.00	27.52	6
ATOM	3406	OG	SER	A	417	1.734	16.874	18.237	1.00	32.78	8
ATOM	3407	C	SER	A	417	2.585	18.852	16.929	1.00	23.50	6
ATOM	3408	O	SER	A	417	1.821	19.541	16.258	1.00	23.90	8
ATOM	3409	N	SER	A	418	3.145	19.217	18.073	1.00	23.61	7
ATOM	3410	CA	SER	A	418	2.982	20.541	18.628	1.00	23.56	6
ATOM	3411	CB	SER	A	418	3.247	20.523	20.135	1.00	24.90	6
ATOM	3412	OG	SER	A	418	4.660	20.195	20.198	1.00	27.24	8
ATOM	3413	C	SER	A	418	3.988	21.525	18.023	1.00	23.37	6
ATOM	3414	O	SER	A	418	3.995	22.714	18.503	1.00	23.96	8
ATOM	3415	N	VAL	A	419	4.894	21.195	17.094	1.00	22.44	7
ATOM	3416	CA	VAL	A	419	5.793	22.233	16.490	1.00	21.33	6
ATOM	3417	CB	VAL	A	419	7.278	22.269	16.815	1.00	19.53	6
ATOM	3418	CG1	VAL	A	419	8.070	23.317	16.038	1.00	15.95	6
ATOM	3419	CG2	VAL	A	419	7.558	22.527	18.315	1.00	18.97	6
ATOM	3420	C	VAL	A	419	5.477	21.951	14.988	1.00	20.67	6
ATOM	3421	O	VAL	A	419	5.911	20.939	14.404	1.00	20.45	8
ATOM	3422	N	ALA	A	420	4.616	22.803	14.400	1.00	20.01	7
ATOM	3423	CA	ALA	A	420	4.174	22.558	13.017	1.00	19.28	6
ATOM	3424	CB	ALA	A	420	3.189	23.619	12.527	1.00	19.92	6
ATOM	3425	C	ALA	A	420	5.329	22.464	12.050	1.00	18.43	6
ATOM	3426	O	ALA	A	420	6.221	23.297	12.166	1.00	18.43	8
ATOM	3427	N	ASN	A	421	5.312	21.471	11.161	1.00	17.67	7
ATOM	3428	CA	ASN	A	421	6.356	21.242	10.168	1.00	16.69	6
ATOM	3429	CB	ASN	A	421	6.537	22.436	9.204	1.00	19.20	6
ATOM	3430	CG	ASN	A	421	5.312	22.617	8.330	1.00	21.29	6
ATOM	3431	OD1	ASN	A	421	4.586	21.711	7.966	1.00	22.05	8
ATOM	3432	ND2	ASN	A	421	5.028	23.853	7.994	1.00	23.75	7
ATOM	3433	C	ASN	A	421	7.760	20.891	10.703	1.00	15.64	6
ATOM	3434	O	ASN	A	421	8.711	20.946	9.931	1.00	15.23	8
ATOM	3435	N	SER	A	422	7.882	20.479	11.947	1.00	14.78	7
ATOM	3436	CA	SER	A	422	9.140	20.088	12.542	1.00	14.31	6
ATOM	3437	CB	SER	A	422	9.064	20.137	14.071	1.00	14.37	6
ATOM	3438	OG	SER	A	422	7.990	19.345	14.623	1.00	13.80	8
ATOM	3439	C	SER	A	422	9.518	18.705	12.009	1.00	13.67	6
ATOM	3440	O	SER	A	422	8.713	17.932	11.459	1.00	13.79	8
ATOM	3441	N	GLY	A	423	10.797	18.389	12.161	1.00	12.94	7
ATOM	3442	CA	GLY	A	423	11.329	17.086	11.679	1.00	12.05	6
ATOM	3443	C	GLY	A	423	12.546	17.472	10.825	1.00	11.56	6
ATOM	3444	O	GLY	A	423	12.532	18.566	10.232	1.00	11.46	8
ATOM	3445	N	LEU	A	424	13.562	16.612	10.738	1.00	10.94	7
ATOM	3446	CA	LEU	A	424	14.738	16.900	9.939	1.00	10.33	6
ATOM	3447	CB	LEU	A	424	15.547	18.024	10.607	1.00	7.87	6
ATOM	3448	CG	LEU	A	424	16.337	17.716	11.885	1.00	8.31	6
ATOM	3449	CD1	LEU	A	424	17.570	16.854	11.716	1.00	6.65	6
ATOM	3450	CD2	LEU	A	424	16.682	19.107	12.547	1.00	8.33	6
ATOM	3451	C	LEU	A	424	15.577	15.630	9.701	1.00	10.11	6
ATOM	3452	O	LEU	A	424	15.448	14.626	10.407	1.00	10.06	8
ATOM	3453	N	ALA	A	425	16.469	15.658	8.706	1.00	9.69	7
ATOM	3454	CA	ALA	A	425	17.366	14.563	8.361	1.00	9.38	6
ATOM	3455	CB	ALA	A	425	16.885	13.742	7.143	1.00	6.73	6
ATOM	3456	C	ALA	A	425	18.723	15.226	8.124	1.00	9.43	6
ATOM	3457	O	ALA	A	425	18.868	16.069	7.188	1.00	9.26	8
ATOM	3458	N	ALA	A	426	19.705	14.875	8.971	1.00	9.31	7
ATOM	3459	CA	ALA	A	426	21.016	15.474	8.873	1.00	9.28	6
ATOM	3460	CB	ALA	A	426	21.436	16.104	10.234	1.00	9.50	6
ATOM	3461	C	ALA	A	426	22.032	14.435	8.414	1.00	9.49	6
ATOM	3462	O	ALA	A	426	21.989	13.294	8.823	1.00	9.20	8
ATOM	3463	N	LEU	A	427	22.965	14.846	7.581	1.00	9.84	7
ATOM	3464	CA	LEU	A	427	24.057	14.016	7.090	1.00	10.53	6
ATOM	3465	CB	LEU	A	427	23.734	13.630	5.656	1.00	11.90	6
ATOM	3466	CG	LEU	A	427	23.768	12.238	5.062	1.00	13.08	6
ATOM	3467	CD1	LEU	A	427	23.577	11.104	6.058	1.00	11.36	6
ATOM	3468	CD2	LEU	A	427	22.742	12.170	3.946	1.00	12.77	6
ATOM	3469	C	LEU	A	427	25.327	14.877	7.098	1.00	10.73	6
ATOM	3470	O	LEU	A	427	25.367	16.056	6.700	1.00	10.84	8
ATOM	3471	N	ILE	A	428	26.460	14.404	7.520	1.00	10.83	7
ATOM	3472	CA	ILE	A	428	27.758	15.045	7.515	1.00	11.06	6
ATOM	3473	CB	ILE	A	428	28.190	15.609	8.889	1.00	11.39	6
ATOM	3474	CG2	ILE	A	428	27.289	16.778	9.305	1.00	10.87	6
ATOM	3475	CG1	ILE	A	428	28.230	14.513	9.993	1.00	9.31	6
ATOM	3476	CD1	ILE	A	428	28.912	15.018	11.283	1.00	8.18	6
ATOM	3477	C	ILE	A	428	28.779	14.006	6.996	1.00	11.33	6
ATOM	3478	O	ILE	A	428	28.561	12.780	7.210	1.00	11.63	8
ATOM	3479	N	THR	A	429	29.881	14.325	6.326	1.00	11.15	7
ATOM	3480	CA	THR	A	429	30.873	13.403	5.891	1.00	10.98	6
ATOM	3481	CB	THR	A	429	31.176	13.138	4.393	1.00	11.90	6
ATOM	3482	OG1	THR	A	429	30.085	13.558	3.592	1.00	14.12	8
ATOM	3483	CG2	THR	A	429	31.612	11.738	4.125	1.00	8.62	6
ATOM	3484	C	THR	A	429	32.246	14.119	6.111	1.00	10.97	6
ATOM	3485	O	THR	A	429	32.413	15.275	5.717	1.00	10.27	8
ATOM	3486	N	ASP	A	430	33.213	13.328	6.605	1.00	11.50	7
ATOM	3487	CA	ASP	A	430	34.540	13.968	6.672	1.00	11.94	6
ATOM	3488	CB	ASP	A	430	35.391	13.652	7.861	1.00	11.35	6
ATOM	3489	CG	ASP	A	430	35.704	12.175	7.893	1.00	12.16	6
ATOM	3490	OD1	ASP	A	430	34.941	11.410	7.236	1.00	12.11	8
ATOM	3491	OD2	ASP	A	430	36.676	11.784	8.551	1.00	10.98	8
ATOM	3492	C	ASP	A	430	35.289	13.562	5.390	1.00	12.62	6
ATOM	3493	O	ASP	A	430	36.452	13.961	5.293	1.00	12.99	8
ATOM	3494	N	GLY	A	431	34.710	12.876	4.425	1.00	12.92	7
ATOM	3495	CA	GLY	A	431	35.369	12.496	3.173	1.00	13.60	6
ATOM	3496	C	GLY	A	431	34.447	12.693	1.981	1.00	13.93	6
ATOM	3497	O	GLY	A	431	33.681	13.671	1.929	1.00	13.86	8
ATOM	3498	N	PRO	A	432	34.509	11.820	0.999	1.00	14.36	7

ATOM	3499	CD	PRO A 432	35.409	10.665	0.884	1.00	14.46	6
ATOM	3500	CA	PRO A 432	33.653	11.935	-0.199	1.00	14.68	6
ATOM	3501	CB	PRO A 432	34.035	10.827	-1.190	1.00	14.46	6
ATOM	3502	CG	PRO A 432	35.224	10.168	-0.544	1.00	14.43	6
ATOM	3503	C	PRO A 432	32.163	11.902	0.220	1.00	14.96	6
ATOM	3504	O	PRO A 432	31.795	11.354	1.273	1.00	14.84	8
ATOM	3505	N	GLY A 433	31.312	12.512	-0.641	1.00	15.15	7
ATOM	3506	CA	GLY A 433	29.882	12.569	-0.450	1.00	15.39	6
ATOM	3507	C	GLY A 433	29.192	11.254	-0.788	1.00	15.65	6
ATOM	3508	O	GLY A 433	29.814	10.259	-1.188	1.00	15.62	8
ATOM	3509	N	GLY A 434	27.885	11.213	-0.658	1.00	15.83	7
ATOM	3510	CA	GLY A 434	27.160	9.983	-0.950	1.00	15.94	6
ATOM	3511	C	GLY A 434	25.733	10.059	-0.444	1.00	15.96	6
ATOM	3512	O	GLY A 434	25.263	11.153	-0.176	1.00	16.25	8
ATOM	3513	N	ALA A 435	25.080	8.925	-0.297	1.00	15.72	7
ATOM	3514	CA	ALA A 435	23.722	8.872	0.128	1.00	15.72	6
ATOM	3515	CB	ALA A 435	22.858	8.337	-1.047	1.00	15.08	6
ATOM	3516	C	ALA A 435	23.470	7.942	1.309	1.00	15.68	6
ATOM	3517	O	ALA A 435	24.260	7.007	1.516	1.00	15.51	8
ATOM	3518	N	LYS A 436	22.366	8.252	2.019	1.00	15.52	7
ATOM	3519	CA	LYS A 436	21.990	7.383	3.119	1.00	15.58	6
ATOM	3520	CB	LYS A 436	22.566	7.682	4.490	1.00	15.09	6
ATOM	3521	CG	LYS A 436	22.500	6.476	5.442	1.00	14.85	6
ATOM	3522	CD	LYS A 436	23.071	6.769	6.810	1.00	13.83	6
ATOM	3523	CE	LYS A 436	24.448	7.441	6.784	1.00	12.21	6
ATOM	3524	NZ	LYS A 436	25.498	6.400	6.652	1.00	11.33	7
ATOM	3525	C	LYS A 436	20.447	7.396	3.179	1.00	15.62	6
ATOM	3526	O	LYS A 436	19.778	8.405	3.060	1.00	15.33	8
ATOM	3527	N	ARG A 437	19.931	6.177	3.314	1.00	15.95	7
ATOM	3528	CA	ARG A 437	18.502	5.972	3.422	1.00	16.36	6
ATOM	3529	CB	ARG A 437	17.965	4.624	2.977	1.00	23.29	6
ATOM	3530	CG	ARG A 437	17.573	4.499	1.510	1.00	29.80	6
ATOM	3531	CD	ARG A 437	16.656	3.293	1.407	1.00	35.68	6
ATOM	3532	NE	ARG A 437	15.201	3.525	1.319	1.00	40.60	7
ATOM	3533	CZ	ARG A 437	14.309	2.734	1.964	1.00	42.03	6
ATOM	3534	NH1	ARG A 437	14.735	1.740	2.755	1.00	42.08	7
ATOM	3535	NH2	ARG A 437	13.005	2.950	1.814	1.00	42.49	7
ATOM	3536	C	ARG A 437	18.202	6.050	4.911	1.00	15.94	6
ATOM	3537	O	ARG A 437	18.833	5.318	5.678	1.00	15.62	8
ATOM	3538	N	MET A 438	17.303	6.932	5.265	1.00	15.86	7
ATOM	3539	CA	MET A 438	17.019	7.059	6.722	1.00	15.87	6
ATOM	3540	CB	MET A 438	17.846	8.236	7.242	1.00	16.35	6
ATOM	3541	CG	MET A 438	19.360	8.200	7.266	1.00	15.99	6
ATOM	3542	SD	MET A 438	20.172	9.634	7.987	1.00	16.66	16
ATOM	3543	CE	MET A 438	19.698	10.989	6.970	1.00	14.67	6
ATOM	3544	C	MET A 438	15.525	7.205	6.983	1.00	15.63	6
ATOM	3545	O	MET A 438	14.774	7.662	6.109	1.00	15.49	8
ATOM	3546	N	TYR A 439	15.065	6.827	8.145	1.00	15.53	7
ATOM	3547	CA	TYR A 439	13.699	6.862	8.590	1.00	15.72	6
ATOM	3548	CB	TYR A 439	13.484	5.632	9.498	1.00	15.96	6
ATOM	3549	CG	TYR A 439	12.110	5.576	10.071	1.00	16.56	6
ATOM	3550	CD1	TYR A 439	11.044	5.338	9.188	1.00	17.21	6
ATOM	3551	CE1	TYR A 439	9.728	5.283	9.611	1.00	17.34	6
ATOM	3552	CD2	TYR A 439	11.815	5.768	11.397	1.00	16.76	6
ATOM	3553	CE2	TYR A 439	10.514	5.667	11.875	1.00	17.07	6
ATOM	3554	CZ	TYR A 439	9.490	5.433	10.974	1.00	17.36	6
ATOM	3555	OH	TYR A 439	8.184	5.345	11.408	1.00	17.36	8
ATOM	3556	C	TYR A 439	13.404	8.144	9.357	1.00	15.81	6
ATOM	3557	O	TYR A 439	13.994	8.512	10.382	1.00	15.50	8
ATOM	3558	N	VAL A 440	12.407	8.831	8.856	1.00	16.08	7
ATOM	3559	CA	VAL A 440	11.897	10.144	9.350	1.00	16.61	6
ATOM	3560	CB	VAL A 440	11.999	10.905	7.980	1.00	16.77	6
ATOM	3561	CG1	VAL A 440	10.764	11.601	7.561	1.00	17.08	6
ATOM	3562	CG2	VAL A 440	13.263	11.754	8.026	1.00	15.70	6
ATOM	3563	C	VAL A 440	10.554	10.106	10.031	1.00	17.07	6
ATOM	3564	O	VAL A 440	10.014	11.040	10.625	1.00	16.85	8
ATOM	3565	N	GLY A 441	9.900	8.915	9.995	1.00	17.47	7
ATOM	3566	CA	GLY A 441	8.607	8.729	10.597	1.00	18.13	6
ATOM	3567	C	GLY A 441	7.583	8.699	9.476	1.00	18.60	6
ATOM	3568	O	GLY A 441	7.616	9.450	8.514	1.00	18.47	8
ATOM	3569	N	ARG A 442	6.636	7.793	9.673	1.00	19.21	7
ATOM	3570	CA	ARG A 442	5.540	7.559	8.739	1.00	19.79	6
ATOM	3571	CB	ARG A 442	4.804	6.264	9.145	1.00	27.13	6
ATOM	3572	CG	ARG A 442	3.910	5.788	8.008	1.00	34.25	6
ATOM	3573	CD	ARG A 442	3.727	4.252	7.911	1.00	40.05	6
ATOM	3574	NE	ARG A 442	3.027	3.980	6.634	1.00	44.01	7
ATOM	3575	CZ	ARG A 442	1.896	3.329	6.388	1.00	46.30	6
ATOM	3576	NH1	ARG A 442	1.175	2.772	7.381	1.00	47.10	7
ATOM	3577	NH2	ARG A 442	1.446	3.253	5.119	1.00	46.98	7
ATOM	3578	C	ARG A 442	4.586	8.725	8.657	1.00	19.53	6
ATOM	3579	O	ARG A 442	3.955	9.003	7.621	1.00	19.67	8
ATOM	3580	N	GLN A 443	4.479	9.544	9.684	1.00	19.05	7
ATOM	3581	CA	GLN A 443	3.607	10.709	9.658	1.00	18.69	6
ATOM	3582	CB	GLN A 443	3.431	11.246	11.093	1.00	21.29	6
ATOM	3583	CG	GLN A 443	4.808	11.675	11.634	1.00	23.26	6
ATOM	3584	CD	GLN A 443	5.581	10.603	12.390	1.00	24.64	6
ATOM	3585	OE1	GLN A 443	5.631	9.402	12.134	1.00	24.10	8
ATOM	3586	NE2	GLN A 443	6.316	11.066	13.438	1.00	25.50	7
ATOM	3587	C	GLN A 443	4.115	11.806	8.734	1.00	18.06	6
ATOM	3588	O	GLN A 443	3.414	12.798	8.501	1.00	17.90	8
ATOM	3589	N	ASN A 444	5.307	11.714	8.193	1.00	17.51	7
ATOM	3590	CA	ASN A 444	5.897	12.636	7.253	1.00	16.84	6
ATOM	3591	CB	ASN A 444	7.400	12.828	7.563	1.00	14.89	6
ATOM	3592	CG	ASN A 444	7.497	13.458	8.951	1.00	15.66	6
ATOM	3593	OD1	ASN A 444	6.765	14.374	9.269	1.00	13.70	8
ATOM	3594	ND2	ASN A 444	8.368	12.974	9.818	1.00	15.53	7
ATOM	3595	C	ASN A 444	5.814	12.078	5.820	1.00	16.45	6
ATOM	3596	O	ASN A 444	6.396	12.716	4.943	1.00	16.24	8
ATOM	3597	N	ALA A 445	5.196	10.917	5.640	1.00	16.01	7
ATOM	3598	CA	ALA A 445	5.075	10.268	4.345	1.00	16.03	6
ATOM	3599	CB	ALA A 445	4.109	9.075	4.403	1.00	15.55	6
ATOM	3600	C	ALA A 445	4.572	11.159	3.208	1.00	15.90	6
ATOM	3601	O	ALA A 445	3.624	11.896	3.441	1.00	15.97	8
ATOM	3602	N	GLY A 446	5.165	11.130	2.010	1.00	15.77	7
ATOM	3603	CA	GLY A 446	4.752	11.944	0.885	1.00	15.36	6
ATOM	3604	C	GLY A 446	5.207	13.378	0.863	1.00	15.20	6

SUBSTITUTE SHEET (RULE 26)

Appendix 1

ATOM	3605	O	GLY	A	446	4.924	14.124	-0.086	1.00	15.33	8
ATOM	3606	N	GLU	A	447	5.963	13.897	1.827	1.00	14.73	7
ATOM	3607	CA	GLU	A	447	6.387	15.280	1.807	1.00	14.28	6
ATOM	3608	CB	GLU	A	447	6.706	15.729	3.264	1.00	14.39	6
ATOM	3609	CG	GLU	A	447	5.389	15.838	4.018	1.00	13.77	6
ATOM	3610	CD	GLU	A	447	5.715	15.992	5.455	1.00	15.49	6
ATOM	3611	OE1	GLU	A	447	6.875	16.135	5.959	1.00	15.55	8
ATOM	3612	OE2	GLU	A	447	4.721	16.000	6.203	1.00	15.31	8
ATOM	3613	C	GLU	A	447	7.644	15.680	1.041	1.00	13.72	6
ATOM	3614	O	GLU	A	447	8.494	14.838	0.929	1.00	13.70	8
ATOM	3615	N	THR	A	448	7.703	16.924	0.604	1.00	13.28	7
ATOM	3616	CA	THR	A	448	8.904	17.386	-0.059	1.00	13.29	6
ATOM	3617	CB	THR	A	448	8.681	18.432	-1.179	1.00	14.50	6
ATOM	3618	OG1	THR	A	448	7.898	17.829	-2.231	1.00	16.23	8
ATOM	3619	CG2	THR	A	448	9.966	18.972	-1.787	1.00	12.12	6
ATOM	3620	C	THR	A	448	9.826	18.047	0.994	1.00	12.85	6
ATOM	3621	O	THR	A	448	9.440	19.036	1.627	1.00	12.61	8
ATOM	3622	N	TRP	A	449	11.021	17.500	1.176	1.00	12.53	7
ATOM	3623	CA	TRP	A	449	12.011	18.069	2.095	1.00	12.56	6
ATOM	3624	CB	TRP	A	449	12.564	16.992	3.035	1.00	9.67	6
ATOM	3625	CG	TRP	A	449	11.619	16.660	4.133	1.00	9.33	6
ATOM	3626	CD2	TRP	A	449	11.959	16.118	5.402	1.00	8.65	6
ATOM	3627	CE2	TRP	A	449	10.762	15.974	6.129	1.00	9.46	6
ATOM	3628	CE3	TRP	A	449	13.161	15.756	6.000	1.00	9.00	6
ATOM	3629	CD1	TRP	A	449	10.237	16.787	4.154	1.00	9.60	6
ATOM	3630	NE1	TRP	A	449	9.710	16.414	5.351	1.00	9.39	7
ATOM	3631	CZ2	TRP	A	449	10.730	15.465	7.438	1.00	9.93	6
ATOM	3632	CZ3	TRP	A	449	13.135	15.216	7.286	1.00	7.79	6
ATOM	3633	CH2	TRP	A	449	11.953	15.068	7.958	1.00	8.43	6
ATOM	3634	C	TRP	A	449	13.168	18.721	1.320	1.00	12.82	6
ATOM	3635	O	TRP	A	449	13.563	18.178	0.275	1.00	12.56	8
ATOM	3636	N	HIS	A	450	13.727	19.836	1.779	1.00	13.04	7
ATOM	3637	CA	HIS	A	450	14.852	20.452	1.046	1.00	13.34	6
ATOM	3638	CB	HIS	A	450	14.296	21.682	0.331	1.00	14.62	6
ATOM	3639	CG	HIS	A	450	14.289	22.883	1.191	1.00	17.87	6
ATOM	3640	CD2	HIS	A	450	14.886	24.101	1.061	1.00	19.94	6
ATOM	3641	ND1	HIS	A	450	13.580	22.945	2.378	1.00	20.15	7
ATOM	3642	CE1	HIS	A	450	13.725	24.121	2.973	1.00	20.37	6
ATOM	3643	NE2	HIS	A	450	14.513	24.848	2.189	1.00	21.15	7
ATOM	3644	C	HIS	A	450	16.040	20.732	1.990	1.00	13.31	6
ATOM	3645	O	HIS	A	450	15.781	20.891	3.188	1.00	13.10	8
ATOM	3646	N	ASP	A	451	17.301	20.807	1.520	1.00	13.09	7
ATOM	3647	CA	ASP	A	451	18.454	21.055	2.375	1.00	12.90	6
ATOM	3648	CB	ASP	A	451	19.697	20.740	1.535	1.00	10.89	6
ATOM	3649	CG	ASP	A	451	21.008	21.054	2.191	1.00	10.97	6
ATOM	3650	OD1	ASP	A	451	20.976	21.407	3.391	1.00	9.94	8
ATOM	3651	OD2	ASP	A	451	22.111	20.978	1.592	1.00	11.53	8
ATOM	3652	C	ASP	A	451	18.403	22.477	2.886	1.00	13.21	6
ATOM	3653	O	ASP	A	451	18.643	23.419	2.089	1.00	13.23	8
ATOM	3654	N	ILE	A	452	18.095	22.816	4.131	1.00	13.24	7
ATOM	3655	CA	ILE	A	452	18.064	24.235	4.561	1.00	13.53	6
ATOM	3656	CB	ILE	A	452	17.466	24.250	5.994	1.00	13.03	6
ATOM	3657	CG2	ILE	A	452	18.495	23.677	6.964	1.00	11.72	6
ATOM	3658	CG1	ILE	A	452	17.009	25.640	6.443	1.00	14.27	6
ATOM	3659	CD1	ILE	A	452	16.275	25.551	7.802	1.00	14.37	6
ATOM	3660	C	ILE	A	452	19.424	24.911	4.512	1.00	13.90	6
ATOM	3661	O	ILE	A	452	19.482	26.146	4.529	1.00	13.78	8
ATOM	3662	N	THR	A	453	20.598	24.254	4.476	1.00	14.31	7
ATOM	3663	CA	THR	A	453	21.885	24.911	4.427	1.00	14.90	6
ATOM	3664	CB	THR	A	453	23.063	23.977	4.697	1.00	12.74	6
ATOM	3665	OG1	THR	A	453	23.194	23.019	3.614	1.00	12.38	8
ATOM	3666	CG2	THR	A	453	22.905	23.215	6.001	1.00	12.32	6
ATOM	3667	C	THR	A	453	22.184	25.480	3.030	1.00	15.80	6
ATOM	3668	O	THR	A	453	23.073	26.280	2.774	1.00	15.75	8
ATOM	3669	N	GLY	A	454	21.475	24.968	2.016	1.00	16.49	7
ATOM	3670	CA	GLY	A	454	21.614	25.345	0.622	1.00	16.88	6
ATOM	3671	C	GLY	A	454	22.752	24.598	-0.055	1.00	17.42	6
ATOM	3672	O	GLY	A	454	22.967	24.858	-1.237	1.00	17.55	8
ATOM	3673	N	ASN	A	455	23.496	23.700	0.568	1.00	17.75	7
ATOM	3674	CA	ASN	A	455	24.590	22.992	-0.090	1.00	18.19	6
ATOM	3675	CB	ASN	A	455	25.375	22.188	0.928	1.00	17.61	6
ATOM	3676	CG	ASN	A	455	26.145	23.158	1.831	1.00	19.02	6
ATOM	3677	OD1	ASN	A	455	26.584	24.193	1.296	1.00	20.84	8
ATOM	3678	ND2	ASN	A	455	26.283	22.827	3.103	1.00	17.34	7
ATOM	3679	C	ASN	A	455	24.050	22.108	-1.217	1.00	18.75	6
ATOM	3680	O	ASN	A	455	24.847	21.968	-2.160	1.00	18.87	8
ATOM	3681	N	ARG	A	456	22.843	21.544	-1.115	1.00	18.85	7
ATOM	3682	CA	ARG	A	456	22.300	20.763	-2.215	1.00	19.42	6
ATOM	3683	CB	ARG	A	456	22.051	19.313	-1.853	1.00	21.00	6
ATOM	3684	CG	ARG	A	456	23.405	18.670	-1.612	1.00	22.06	6
ATOM	3685	CD	ARG	A	456	23.079	17.230	-1.408	1.00	24.47	6
ATOM	3686	NE	ARG	A	456	22.752	16.607	-2.676	1.00	27.86	7
ATOM	3687	CZ	ARG	A	456	23.472	16.017	-3.613	1.00	29.09	6
ATOM	3688	NH1	ARG	A	456	22.809	15.484	-4.631	1.00	29.42	7
ATOM	3689	NH2	ARG	A	456	24.789	15.821	-3.652	1.00	30.25	7
ATOM	3690	C	ARG	A	456	20.994	21.388	-2.721	1.00	19.69	6
ATOM	3691	O	ARG	A	456	20.182	21.809	-1.881	1.00	19.86	8
ATOM	3692	N	SER	A	457	20.777	21.515	-4.032	1.00	19.78	7
ATOM	3693	CA	SER	A	457	19.533	22.134	-4.501	1.00	19.97	6
ATOM	3694	CB	SER	A	457	19.748	23.040	-5.741	1.00	20.18	6
ATOM	3695	OG	SER	A	457	20.301	22.068	-6.668	1.00	20.86	8
ATOM	3696	C	SER	A	457	18.439	21.136	-4.883	1.00	19.94	6
ATOM	3697	O	SER	A	457	17.317	21.592	-5.183	1.00	20.17	8
ATOM	3698	N	GLU	A	458	18.708	19.841	-4.835	1.00	19.72	7
ATOM	3699	CA	GLU	A	458	17.687	18.883	-5.161	1.00	19.82	6
ATOM	3700	CB	GLU	A	458	18.321	17.611	-5.803	1.00	24.71	6
ATOM	3701	CG	GLU	A	458	17.134	17.001	-6.543	1.00	31.90	6
ATOM	3702	CD	GLU	A	458	17.152	15.635	-7.168	1.00	36.18	6
ATOM	3703	OE1	GLU	A	458	18.250	15.229	-7.681	1.00	38.60	8
ATOM	3704	OE2	GLU	A	458	16.057	14.979	-7.142	1.00	38.01	8
ATOM	3705	C	GLU	A	458	16.850	18.407	-3.978	1.00	19.28	6
ATOM	3706	O	GLU	A	458	17.375	17.778	-3.068	1.00	19.23	8
ATOM	3707	N	PRO	A	459	15.545	18.628	-4.028	1.00	18.75	7
ATOM	3708	CD	PRO	A	459	14.893	19.401	-5.083	1.00	18.49	6
ATOM	3709	CA	PRO	A	459	14.611	18.231	-2.974	1.00	18.56	6
ATOM	3710	CB	PRO	A	459	13.270	18.916	-3.298	1.00	18.40	6

ATOM	3711	CG	PRO	A	459	13.637	19.885	-4.393	1.00	18.37	6
ATOM	3712	C	PRO	A	459	14.504	16.723	-2.839	1.00	18.47	6
ATOM	3713	O	PRO	A	459	14.829	15.979	-3.780	1.00	18.68	8
ATOM	3714	N	VAL	A	460	14.113	16.146	-1.728	1.00	18.24	7
ATOM	3715	CA	VAL	A	460	13.987	14.691	-1.504	1.00	18.19	6
ATOM	3716	CB	VAL	A	460	14.906	14.168	-0.379	1.00	17.56	6
ATOM	3717	CG1	VAL	A	460	14.739	12.685	-0.076	1.00	17.48	6
ATOM	3718	CG2	VAL	A	460	16.371	14.396	-0.750	1.00	17.31	6
ATOM	3719	C	VAL	A	460	12.528	14.396	-1.209	1.00	18.23	6
ATOM	3720	O	VAL	A	460	11.892	15.157	-0.428	1.00	18.51	8
ATOM	3721	N	VAL	A	461	11.894	13.362	-1.798	1.00	18.03	7
ATOM	3722	CA	VAL	A	461	10.468	13.105	-1.458	1.00	17.66	6
ATOM	3723	CB	VAL	A	461	9.584	12.863	-2.709	1.00	17.06	6
ATOM	3724	CG1	VAL	A	461	8.143	12.564	-2.256	1.00	16.42	6
ATOM	3725	CG2	VAL	A	461	9.629	14.023	-3.678	1.00	15.12	6
ATOM	3726	C	VAL	A	461	10.418	11.943	-0.456	1.00	17.45	6
ATOM	3727	O	VAL	A	461	11.046	10.893	-0.596	1.00	17.01	8
ATOM	3728	N	ILE	A	462	9.707	12.111	0.647	1.00	17.69	7
ATOM	3729	CA	ILE	A	462	9.596	11.050	1.642	1.00	18.12	6
ATOM	3730	CB	ILE	A	462	9.212	11.549	3.046	1.00	15.81	6
ATOM	3731	CG2	ILE	A	462	9.222	10.334	3.984	1.00	15.11	6
ATOM	3732	CG1	ILE	A	462	10.089	12.691	3.597	1.00	13.00	6
ATOM	3733	CD1	ILE	A	462	11.575	12.439	3.642	1.00	9.27	6
ATOM	3734	C	ILE	A	462	8.554	10.036	1.116	1.00	18.85	6
ATOM	3735	O	ILE	A	462	7.432	10.390	0.717	1.00	18.67	8
ATOM	3736	N	ASN	A	463	8.922	8.755	1.138	1.00	19.55	7
ATOM	3737	CA	ASN	A	463	8.090	7.650	0.672	1.00	20.49	6
ATOM	3738	CB	ASN	A	463	8.960	6.443	0.342	1.00	20.20	6
ATOM	3739	CG	ASN	A	463	9.411	5.430	1.361	1.00	21.59	6
ATOM	3740	OD1	ASN	A	463	9.117	5.376	2.570	1.00	22.11	8
ATOM	3741	ND2	ASN	A	463	10.221	4.455	0.904	1.00	19.99	7
ATOM	3742	C	ASN	A	463	6.975	7.297	1.630	1.00	21.45	6
ATOM	3743	O	ASN	A	463	6.884	7.742	2.770	1.00	21.42	8
ATOM	3744	N	SER	A	464	6.070	6.390	1.173	1.00	22.31	7
ATOM	3745	CA	SER	A	464	4.877	5.971	1.916	1.00	22.97	6
ATOM	3746	CB	SER	A	464	3.915	5.159	1.024	1.00	23.92	6
ATOM	3747	OG	SER	A	464	4.365	3.841	0.731	1.00	25.69	8
ATOM	3748	C	SER	A	464	5.187	5.303	3.248	1.00	23.29	6
ATOM	3749	O	SER	A	464	4.319	5.400	4.131	1.00	23.52	8
ATOM	3750	N	GLU	A	465	6.344	4.722	3.486	1.00	23.46	7
ATOM	3751	CA	GLU	A	465	6.814	4.134	4.708	1.00	23.73	6
ATOM	3752	CB	GLU	A	465	7.931	3.164	4.313	1.00	29.98	6
ATOM	3753	CG	GLU	A	465	7.852	1.671	4.515	1.00	35.99	6
ATOM	3754	CD	GLU	A	465	6.542	1.117	3.976	1.00	39.49	6
ATOM	3755	OE1	GLU	A	465	6.407	1.177	2.734	1.00	41.43	8
ATOM	3756	OE2	GLU	A	465	5.709	0.684	4.812	1.00	41.76	8
ATOM	3757	C	GLU	A	465	7.511	5.095	5.721	1.00	23.27	6
ATOM	3758	O	GLU	A	465	7.857	4.672	6.848	1.00	23.24	8
ATOM	3759	N	GLY	A	466	7.744	6.345	5.324	1.00	22.53	7
ATOM	3760	CA	GLY	A	466	8.436	7.317	6.135	1.00	21.95	6
ATOM	3761	C	GLY	A	466	9.969	7.245	5.909	1.00	21.47	6
ATOM	3762	O	GLY	A	466	10.728	7.644	6.820	1.00	21.33	8
ATOM	3763	N	TRP	A	467	10.441	6.770	4.751	1.00	20.79	7
ATOM	3764	CA	TRP	A	467	11.860	6.686	4.486	1.00	20.35	6
ATOM	3765	CB	TRP	A	467	12.439	5.313	4.107	1.00	20.44	6
ATOM	3766	CG	TRP	A	467	12.372	4.283	5.181	1.00	20.04	6
ATOM	3767	CD2	TRP	A	467	13.427	3.771	5.993	1.00	19.41	6
ATOM	3768	CE2	TRP	A	467	12.844	2.826	6.880	1.00	19.61	6
ATOM	3769	CE3	TRP	A	467	14.803	3.987	6.049	1.00	18.58	6
ATOM	3770	CD1	TRP	A	467	11.227	3.633	5.591	1.00	20.26	6
ATOM	3771	NE1	TRP	A	467	11.497	2.779	6.622	1.00	19.67	7
ATOM	3772	CZ2	TRP	A	467	13.593	2.102	7.824	1.00	19.59	6
ATOM	3773	CZ3	TRP	A	467	15.552	3.268	6.997	1.00	20.04	6
ATOM	3774	CH2	TRP	A	467	14.959	2.315	7.868	1.00	19.86	6
ATOM	3775	C	TRP	A	467	12.174	7.631	3.312	1.00	20.06	6
ATOM	3776	O	TRP	A	467	11.355	7.837	2.413	1.00	19.99	8
ATOM	3777	N	GLY	A	468	13.356	8.193	3.372	1.00	19.55	7
ATOM	3778	CA	GLY	A	468	13.838	9.105	2.345	1.00	19.08	6
ATOM	3779	C	GLY	A	468	15.293	8.667	2.044	1.00	18.67	6
ATOM	3780	O	GLY	A	468	15.969	8.121	2.908	1.00	18.51	8
ATOM	3781	N	GLU	A	469	15.761	8.896	0.848	1.00	18.42	7
ATOM	3782	CA	GLU	A	469	17.153	8.577	0.487	1.00	18.35	6
ATOM	3783	CB	GLU	A	469	17.287	7.714	-0.771	1.00	23.55	6
ATOM	3784	CG	GLU	A	469	18.710	7.626	-1.293	1.00	29.59	6
ATOM	3785	CD	GLU	A	469	18.967	7.178	-2.729	1.00	34.28	6
ATOM	3786	OE1	GLU	A	469	19.831	6.252	-2.904	1.00	36.09	8
ATOM	3787	OE2	GLU	A	469	18.340	7.755	-3.681	1.00	35.52	8
ATOM	3788	C	GLU	A	469	17.805	9.964	0.424	1.00	17.57	6
ATOM	3789	O	GLU	A	469	17.555	10.801	-0.433	1.00	17.46	8
ATOM	3790	N	PHE	A	470	18.666	10.297	1.388	1.00	17.09	7
ATOM	3791	CA	PHE	A	470	19.246	11.660	1.415	1.00	16.47	6
ATOM	3792	CB	PHE	A	470	19.076	12.181	2.850	1.00	14.77	6
ATOM	3793	CG	PHE	A	470	17.686	12.126	3.451	1.00	11.90	6
ATOM	3794	CD1	PHE	A	470	17.301	11.041	4.208	1.00	11.94	6
ATOM	3795	CD2	PHE	A	470	16.823	13.197	3.296	1.00	10.16	6
ATOM	3796	CE1	PHE	A	470	16.037	11.030	4.790	1.00	11.36	6
ATOM	3797	CE2	PHE	A	470	15.562	13.155	3.871	1.00	9.61	6
ATOM	3798	CZ	PHE	A	470	15.159	12.069	4.605	1.00	9.27	6
ATOM	3799	C	PHE	A	470	20.682	11.731	0.945	1.00	16.14	6
ATOM	3800	O	PHE	A	470	21.406	10.761	1.154	1.00	16.37	8
ATOM	3801	N	HIS	A	471	21.142	12.807	0.363	1.00	15.78	7
ATOM	3802	CA	HIS	A	471	22.462	13.007	-0.146	1.00	15.69	6
ATOM	3803	CB	HIS	A	471	22.332	13.373	-1.655	1.00	17.00	6
ATOM	3804	CG	HIS	A	471	21.894	12.216	-2.515	1.00	20.58	6
ATOM	3805	CD2	HIS	A	471	22.588	11.406	-3.372	1.00	21.49	6
ATOM	3806	ND1	HIS	A	471	20.560	11.780	-2.567	1.00	22.05	7
ATOM	3807	CE1	HIS	A	471	20.481	10.745	-3.399	1.00	21.74	6
ATOM	3808	NE2	HIS	A	471	21.688	10.491	-3.900	1.00	22.49	7
ATOM	3809	C	HIS	A	471	23.282	14.111	0.504	1.00	15.47	6
ATOM	3810	O	HIS	A	471	22.727	15.102	0.997	1.00	15.28	8
ATOM	3811	N	VAL	A	472	24.618	13.993	0.446	1.00	15.23	7
ATOM	3812	CA	VAL	A	472	25.529	14.978	0.964	1.00	15.01	6
ATOM	3813	CB	VAL	A	472	26.385	14.698	2.271	1.00	16.48	6
ATOM	3814	CG1	VAL	A	472	26.201	15.727	3.368	1.00	15.07	6
ATOM	3815	CG2	VAL	A	472	26.275	13.274	2.750	1.00	17.23	6
ATOM	3816	C	VAL	A	472	26.730	15.205	0.001	1.00	14.42	6

ATOM	3817	O	VAL	A	472	27.246	14.169	-0.462	1.00	14.29	8
ATOM	3818	N	ASN	A	473	27.200	16.444	-0.101	1.00	13.78	7
ATOM	3819	CA	ASN	A	473	28.404	16.662	-0.901	1.00	13.30	6
ATOM	3820	CB	ASN	A	473	28.514	18.108	-1.339	1.00	13.44	6
ATOM	3821	CG	ASN	A	473	27.403	18.519	-2.301	1.00	15.11	6
ATOM	3822	OD1	ASN	A	473	26.781	17.637	-2.882	1.00	15.07	8
ATOM	3823	ND2	ASN	A	473	27.148	19.805	-2.494	1.00	15.52	7
ATOM	3824	C	ASN	A	473	29.633	16.278	-0.086	1.00	12.99	6
ATOM	3825	O	ASN	A	473	29.567	16.164	1.139	1.00	12.88	8
ATOM	3826	N	GLY	A	474	30.792	16.046	-0.723	1.00	12.57	7
ATOM	3827	CA	GLY	A	474	32.004	15.690	0.026	1.00	11.90	6
ATOM	3828	C	GLY	A	474	32.429	16.874	0.897	1.00	11.47	6
ATOM	3829	O	GLY	A	474	32.305	18.054	0.524	1.00	11.68	8
ATOM	3830	N	GLY	A	475	32.940	16.534	2.058	1.00	10.93	7
ATOM	3831	CA	GLY	A	475	33.425	17.392	3.139	1.00	10.37	6
ATOM	3832	C	GLY	A	475	32.350	18.425	3.486	1.00	10.04	6
ATOM	3833	O	GLY	A	475	32.646	19.606	3.607	1.00	9.82	8
ATOM	3834	N	SER	A	476	31.076	17.953	3.556	1.00	9.71	7
ATOM	3835	CA	SER	A	476	29.967	18.862	3.748	1.00	9.25	6
ATOM	3836	CB	SER	A	476	29.330	19.038	2.348	1.00	10.16	6
ATOM	3837	OG	SER	A	476	28.487	20.170	2.237	1.00	11.03	8
ATOM	3838	C	SER	A	476	28.910	18.374	4.718	1.00	8.87	6
ATOM	3839	O	SER	A	476	28.982	17.301	5.311	1.00	8.60	8
ATOM	3840	N	VAL	A	477	27.865	19.207	4.864	1.00	8.73	7
ATOM	3841	CA	VAL	A	477	26.711	18.975	5.699	1.00	8.42	6
ATOM	3842	CB	VAL	A	477	26.705	19.802	7.028	1.00	6.94	6
ATOM	3843	CG1	VAL	A	477	26.953	21.281	6.811	1.00	5.00	6
ATOM	3844	CG2	VAL	A	477	25.389	19.640	7.754	1.00	5.67	6
ATOM	3845	C	VAL	A	477	25.462	19.333	4.887	1.00	8.35	6
ATOM	3846	O	VAL	A	477	25.485	20.297	4.139	1.00	8.26	8
ATOM	3847	N	SER	A	478	24.403	18.567	5.033	1.00	8.45	7
ATOM	3848	CA	SER	A	478	23.087	18.761	4.462	1.00	8.36	6
ATOM	3849	CB	SER	A	478	22.792	17.840	3.254	1.00	8.85	6
ATOM	3850	OG	SER	A	478	23.251	18.520	2.073	1.00	11.98	8
ATOM	3851	C	SER	A	478	22.074	18.493	5.574	1.00	8.16	6
ATOM	3852	O	SER	A	478	22.181	17.527	6.326	1.00	7.79	8
ATOM	3853	N	ILE	A	479	21.114	19.406	5.720	1.00	8.43	7
ATOM	3854	CA	ILE	A	479	20.039	19.323	6.693	1.00	8.49	6
ATOM	3855	CB	ILE	A	479	20.160	20.274	7.884	1.00	8.78	6
ATOM	3856	CG2	ILE	A	479	18.976	19.999	8.846	1.00	6.48	6
ATOM	3857	CG1	ILE	A	479	21.502	20.102	8.647	1.00	8.82	6
ATOM	3858	CD1	ILE	A	479	21.914	21.342	9.399	1.00	7.53	6
ATOM	3859	C	ILE	A	479	18.689	19.539	6.015	1.00	8.75	6
ATOM	3860	O	ILE	A	479	18.346	20.671	5.734	1.00	8.74	8
ATOM	3861	N	TYR	A	480	17.969	18.447	5.791	1.00	9.32	7
ATOM	3862	CA	TYR	A	480	16.682	18.457	5.141	1.00	10.04	6
ATOM	3863	CB	TYR	A	480	16.431	17.093	4.465	1.00	10.47	6
ATOM	3864	CG	TYR	A	480	17.358	16.901	3.299	1.00	11.51	6
ATOM	3865	CD1	TYR	A	480	18.620	16.314	3.605	1.00	12.15	6
ATOM	3866	CE1	TYR	A	480	19.531	16.102	2.589	1.00	12.53	6
ATOM	3867	CD2	TYR	A	480	17.080	17.306	2.001	1.00	11.63	6
ATOM	3868	CE2	TYR	A	480	17.988	17.112	0.996	1.00	12.21	6
ATOM	3869	CZ	TYR	A	480	19.177	16.496	1.294	1.00	12.89	6
ATOM	3870	OH	TYR	A	480	20.153	16.272	0.329	1.00	13.85	8
ATOM	3871	C	TYR	A	480	15.497	18.650	6.064	1.00	10.60	6
ATOM	3872	O	TYR	A	480	15.416	18.002	7.124	1.00	10.50	8
ATOM	3873	N	VAL	A	481	14.597	19.553	5.683	1.00	11.15	7
ATOM	3874	CA	VAL	A	481	13.420	19.904	6.431	1.00	12.11	6
ATOM	3875	CB	VAL	A	481	13.545	21.232	7.239	1.00	10.43	6
ATOM	3876	CG1	VAL	A	481	14.600	21.088	8.319	1.00	10.53	6
ATOM	3877	CG2	VAL	A	481	13.880	22.458	6.409	1.00	7.87	6
ATOM	3878	C	VAL	A	481	12.268	20.106	5.458	1.00	13.24	6
ATOM	3879	O	VAL	A	481	12.481	20.334	4.256	1.00	13.31	8
ATOM	3880	N	GLN	A	482	11.060	20.080	5.969	1.00	14.41	7
ATOM	3881	CA	GLN	A	482	9.911	20.288	5.064	1.00	15.58	6
ATOM	3882	CB	GLN	A	482	8.631	20.328	5.896	1.00	18.30	6
ATOM	3883	CG	GLN	A	482	7.544	21.053	5.090	1.00	23.44	6
ATOM	3884	CD	GLN	A	482	6.745	20.125	4.176	1.00	25.41	6
ATOM	3885	OE1	GLN	A	482	6.283	19.145	4.786	1.00	25.61	8
ATOM	3886	NE2	GLN	A	482	6.540	20.395	2.875	1.00	25.49	7
ATOM	3887	C	GLN	A	482	10.086	21.558	4.246	1.00	16.28	6
ATOM	3888	O	GLN	A	482	10.404	22.646	4.755	1.00	16.41	8
ATOM	3889	N	ARG	A	483	9.856	21.490	2.934	1.00	16.75	7
ATOM	3890	CA	ARG	A	483	9.955	22.625	2.026	1.00	17.07	6
ATOM	3891	CB	ARG	A	483	9.913	22.081	0.609	1.00	18.13	6
ATOM	3892	CG	ARG	A	483	9.621	23.031	-0.524	1.00	19.63	6
ATOM	3893	CD	ARG	A	483	10.817	23.756	-1.071	1.00	22.10	6
ATOM	3894	NE	ARG	A	483	11.199	24.865	-0.224	1.00	24.98	7
ATOM	3895	CZ	ARG	A	483	11.940	25.939	-0.498	1.00	26.41	6
ATOM	3896	NH1	ARG	A	483	12.515	26.296	-1.651	1.00	26.83	7
ATOM	3897	NH2	ARG	A	483	12.081	26.726	0.575	1.00	27.28	7
ATOM	3898	C	ARG	A	483	8.817	23.598	2.308	1.00	17.44	6
ATOM	3899	O	ARG	A	483	9.004	24.833	2.203	1.00	17.63	8
ATOM	3900	OT	ARG	A	483	7.689	23.159	2.631	1.00	18.43	8
ATOM	3901	CA	ION	$	501	44.093	25.586	51.930	1.00	10.30	20
ATOM	3902	CA	ION	$	502	43.109	26.963	43.727	1.00	8.87	20
ATOM	3903	CA	ION	$	503	36.437	9.091	7.752	1.00	19.31	20
ATOM	3904	CA	ION	$	504	5.896	16.803	8.528	1.00	17.57	20
ATOM	3905	OW1	WAT	X	1	46.182	29.694	41.805	1.00	5.00	8
ATOM	3906	OW2	WAT	X	1	39.434	45.537	34.032	1.00	7.97	8
ATOM	3907	OW3	WAT	X	1	35.632	30.198	39.664	1.00	5.16	8
ATOM	3908	OW4	WAT	X	1	31.019	26.580	20.085	1.00	5.00	8
ATOM	3909	OW5	WAT	X	1	34.364	20.929	31.664	1.00	7.18	8
ATOM	3910	OW6	WAT	X	1	24.507	18.918	21.861	1.00	11.20	8
ATOM	3911	OW7	WAT	X	1	38.313	44.279	32.223	1.00	6.82	8
ATOM	3912	OW8	WAT	X	1	39.624	39.129	42.515	1.00	5.00	8
ATOM	3913	OW9	WAT	X	1	30.223	47.484	41.150	1.00	8.45	8
ATOM	3914	OW0	WAT	X	2	35.182	46.470	25.198	1.00	13.57	8
ATOM	3915	OW1	WAT	X	2	39.320	23.655	35.030	1.00	5.58	8
ATOM	3916	OW2	WAT	X	2	39.029	37.148	61.342	1.00	6.00	8
ATOM	3917	OW3	WAT	X	2	31.724	19.710	23.165	1.00	6.36	8
ATOM	3918	OW4	WAT	X	2	5.684	18.660	1.089	1.00	13.82	8
ATOM	3919	OW5	WAT	X	2	38.823	36.243	42.467	1.00	5.27	8
ATOM	3920	OW6	WAT	X	2	37.438	41.652	45.589	1.00	5.00	8
ATOM	3921	OW7	WAT	X	2	14.634	9.750	20.928	1.00	13.75	8
ATOM	3922	OW8	WAT	X	2	38.712	30.913	38.542	1.00	7.22	8

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ATOM	3923	OW9	WAT	X	2	42.991	28.597	56.879	1.00	19.54	8
ATOM	3924	OW0	WAT	X	3	42.416	33.909	17.726	1.00	10.85	8
ATOM	3925	OW1	WAT	X	3	48.842	22.953	44.340	1.00	7.46	8
ATOM	3926	OW2	WAT	X	3	36.038	55.628	43.083	1.00	10.34	8
ATOM	3927	OW3	WAT	X	3	58.570	25.578	42.683	1.00	12.51	8
ATOM	3928	OW4	WAT	X	3	35.732	43.524	49.882	1.00	5.95	8
ATOM	3929	OW5	WAT	X	3	26.190	18.692	1.154	1.00	12.57	8
ATOM	3930	OW6	WAT	X	3	40.723	25.525	46.044	1.00	10.44	8
ATOM	3931	OW7	WAT	X	3	41.640	28.398	45.135	1.00	5.00	8
ATOM	3932	OW8	WAT	X	3	36.546	42.416	33.352	1.00	5.00	8
ATOM	3933	OW9	WAT	X	3	40.987	21.110	52.091	1.00	20.54	8
ATOM	3934	OW0	WAT	X	4	37.695	27.410	12.493	1.00	11.34	8
ATOM	3935	OW1	WAT	X	4	22.844	23.707	36.872	1.00	9.80	8
ATOM	3936	OW2	WAT	X	4	36.012	18.648	48.284	1.00	17.35	8
ATOM	3937	OW3	WAT	X	4	31.899	45.870	33.523	1.00	10.56	8
ATOM	3938	OW4	WAT	X	4	30.501	38.096	33.954	1.00	11.67	8
ATOM	3939	OW5	WAT	X	4	22.073	12.907	32.231	1.00	10.97	8
ATOM	3940	OW6	WAT	X	4	40.488	14.451	42.396	1.00	12.74	8
ATOM	3941	OW7	WAT	X	4	53.405	37.236	44.839	1.00	12.00	8
ATOM	3942	OW8	WAT	X	4	43.396	20.817	52.968	1.00	25.21	8
ATOM	3943	OW9	WAT	X	4	45.712	34.753	17.330	1.00	22.47	8
ATOM	3944	OW0	WAT	X	5	52.299	25.204	54.738	1.00	18.85	8
ATOM	3945	OW1	WAT	X	5	10.464	19.211	8.671	1.00	8.04	8
ATOM	3946	OW2	WAT	X	5	23.407	21.100	30.729	1.00	15.19	8
ATOM	3947	OW3	WAT	X	5	34.672	39.007	47.914	1.00	25.93	8
ATOM	3948	OW4	WAT	X	5	39.440	24.513	6.213	1.00	20.60	8
ATOM	3949	OW5	WAT	X	5	43.207	54.381	40.149	1.00	25.71	8
ATOM	3950	OW6	WAT	X	5	29.887	49.393	26.775	1.00	10.08	8
ATOM	3951	OW7	WAT	X	5	18.296	28.320	27.646	1.00	17.61	8
ATOM	3952	OW8	WAT	X	5	42.657	37.701	31.679	1.00	16.67	8
ATOM	3953	OW9	WAT	X	5	43.242	40.411	24.206	1.00	19.05	8
ATOM	3954	OW0	WAT	X	6	27.361	18.395	39.419	1.00	14.74	8
ATOM	3955	OW1	WAT	X	6	28.339	52.900	35.976	1.00	18.51	8
ATOM	3956	OW2	WAT	X	6	37.756	14.989	39.100	1.00	17.01	8
ATOM	3957	OW3	WAT	X	6	22.840	21.238	35.474	1.00	13.60	8
ATOM	3958	OW4	WAT	X	6	38.940	13.232	9.026	1.00	11.51	8
ATOM	3959	OW5	WAT	X	6	25.342	16.185	20.356	1.00	18.86	8
ATOM	3960	OW6	WAT	X	6	8.361	17.329	8.642	1.00	13.52	8
ATOM	3961	OW7	WAT	X	6	37.794	6.917	7.269	1.00	20.73	8
ATOM	3962	OW8	WAT	X	6	45.060	49.979	33.793	1.00	12.44	8
ATOM	3963	OW9	WAT	X	6	36.427	41.328	48.308	1.00	11.02	8
ATOM	3964	OW0	WAT	X	7	41.263	15.827	37.266	1.00	22.49	8
ATOM	3965	OW1	WAT	X	7	25.131	39.394	49.866	1.00	10.30	8
ATOM	3966	OW2	WAT	X	7	51.050	21.873	54.397	1.00	18.11	8
ATOM	3967	OW3	WAT	X	7	43.851	40.827	26.978	1.00	38.82	8
ATOM	3968	OW4	WAT	X	7	48.952	26.479	52.035	1.00	17.95	8
ATOM	3969	OW5	WAT	X	7	24.717	49.514	27.044	1.00	19.57	8
ATOM	3970	OW6	WAT	X	7	32.551	52.703	28.488	1.00	9.04	8
ATOM	3971	OW7	WAT	X	7	44.885	26.009	54.445	1.00	7.24	8
ATOM	3972	OW8	WAT	X	7	38.325	36.644	45.393	1.00	19.65	8
ATOM	3973	OW9	WAT	X	7	21.609	12.965	20.907	1.00	9.32	8
ATOM	3974	OW0	WAT	X	8	24.711	13.545	20.784	1.00	23.06	8
ATOM	3975	OW1	WAT	X	8	42.374	43.789	25.824	1.00	28.85	8
ATOM	3976	OW2	WAT	X	8	18.586	45.140	20.306	1.00	24.89	8
ATOM	3977	OW3	WAT	X	8	40.969	25.117	33.960	1.00	19.79	8
ATOM	3978	OW4	WAT	X	8	20.088	43.470	17.087	1.00	16.72	8
ATOM	3979	OW5	WAT	X	8	38.467	37.011	11.354	1.00	25.51	8
ATOM	3980	OW6	WAT	X	8	13.729	9.292	-1.198	1.00	18.29	8
ATOM	3981	OW7	WAT	X	8	37.082	34.587	46.550	1.00	20.44	8
ATOM	3982	OW8	WAT	X	8	33.674	26.739	26.941	1.00	37.20	8
ATOM	3983	OW9	WAT	X	8	44.040	39.609	29.378	1.00	15.09	8
ATOM	3984	OW0	WAT	X	9	5.980	17.940	10.956	1.00	15.78	8
ATOM	3985	OW1	WAT	X	9	37.928	39.774	25.743	1.00	20.89	8
ATOM	3986	OW2	WAT	X	9	30.894	54.048	35.873	1.00	15.39	8
ATOM	3987	OW3	WAT	X	9	28.071	34.048	54.110	1.00	17.12	8
ATOM	3988	OW4	WAT	X	9	18.742	28.715	32.238	1.00	16.32	8
ATOM	3989	OW5	WAT	X	9	21.957	31.164	51.343	1.00	17.53	8
ATOM	3990	OW6	WAT	X	9	17.533	31.407	37.350	1.00	18.05	8
ATOM	3991	OW7	WAT	X	9	33.329	26.312	6.343	1.00	16.49	8
ATOM	3992	OW8	WAT	X	9	52.348	36.456	42.429	1.00	22.51	8
ATOM	3993	OW9	WAT	X	9	33.954	32.866	59.563	1.00	24.70	8
ATOM	3994	OW0	WAT	X	10	20.209	19.419	22.073	1.00	15.65	8
ATOM	3995	OW1	WAT	X	10	32.236	16.522	47.616	1.00	20.65	8
ATOM	3996	OW2	WAT	X	10	38.512	27.238	32.842	1.00	17.87	8
ATOM	3997	OW3	WAT	X	10	29.117	21.774	-1.117	1.00	25.65	8
ATOM	3998	OW4	WAT	X	10	36.476	40.547	18.282	1.00	25.86	8
ATOM	3999	OW5	WAT	X	10	18.917	5.144	16.972	1.00	16.17	8
ATOM	4000	OW6	WAT	X	10	23.106	43.383	45.060	1.00	22.47	8
ATOM	4001	OW7	WAT	X	10	27.983	24.700	5.027	1.00	20.60	8
ATOM	4002	OW8	WAT	X	10	34.986	39.869	15.784	1.00	23.70	8
ATOM	4003	OW9	WAT	X	10	5.987	15.831	-1.902	1.00	32.41	8
ATOM	4004	OW0	WAT	X	11	19.643	16.427	-2.512	1.00	35.14	8
ATOM	4005	OW1	WAT	X	11	17.172	19.237	19.676	1.00	29.78	8
ATOM	4006	OW2	WAT	X	11	49.760	21.003	51.233	1.00	9.95	8
ATOM	4007	OW3	WAT	X	11	41.639	31.412	35.004	1.00	25.82	8
ATOM	4008	OW4	WAT	X	11	25.364	51.628	41.093	1.00	29.63	8
ATOM	4009	OW5	WAT	X	11	19.805	23.778	36.990	1.00	33.98	8
ATOM	4010	OW6	WAT	X	11	42.937	27.882	12.460	1.00	37.03	8
ATOM	4011	OW7	WAT	X	11	18.451	29.166	35.333	1.00	27.81	8
ATOM	4012	OW8	WAT	X	11	24.969	26.021	50.840	1.00	26.74	8
ATOM	4013	OW9	WAT	X	11	43.160	54.157	43.072	1.00	23.83	8
ATOM	4014	OW0	WAT	X	12	12.642	37.968	31.162	1.00	65.20	8
ATOM	4015	OW1	WAT	X	12	32.411	23.218	5.138	1.00	18.08	8
ATOM	4016	OW2	WAT	X	12	19.308	3.707	13.407	1.00	50.55	8
ATOM	4017	OW3	WAT	X	12	17.400	20.494	-1.396	1.00	25.22	8
ATOM	4018	OW4	WAT	X	12	38.504	40.778	36.668	1.00	40.52	8
ATOM	4019	OW5	WAT	X	12	46.693	16.740	48.249	1.00	22.77	8
ATOM	4020	OW6	WAT	X	12	44.237	51.654	41.807	1.00	30.69	8
ATOM	4021	OW7	WAT	X	12	29.593	23.052	4.777	1.00	24.15	8
ATOM	4022	OW8	WAT	X	12	25.325	25.894	6.415	1.00	23.43	8
ATOM	4023	OW9	WAT	X	12	37.028	10.496	27.680	1.00	13.65	8
ATOM	4024	OW0	WAT	X	13	15.428	33.267	21.245	1.00	27.08	8
ATOM	4025	OW1	WAT	X	13	32.665	39.080	54.672	1.00	21.60	8
ATOM	4026	OW2	WAT	X	13	46.251	40.891	31.602	1.00	25.79	8
ATOM	4027	OW3	WAT	X	13	38.486	30.224	30.783	1.00	20.87	8
ATOM	4028	OW4	WAT	X	13	42.551	46.583	21.900	1.00	28.42	8

ATOM	4029	OW5	WAT	X	13	13.009	12.182	-4.047	1.00	27.61	8
ATOM	4030	OW6	WAT	X	13	32.756	8.582	1.824	1.00	29.04	8
ATOM	4031	OW7	WAT	X	13	16.249	23.415	-2.919	1.00	36.05	8
ATOM	4032	OW8	WAT	X	13	36.916	46.802	51.068	1.00	13.92	8
ATOM	4033	OW9	WAT	X	13	51.456	45.867	53.043	1.00	27.25	8
ATOM	4034	OW0	WAT	X	14	44.576	23.979	15.915	1.00	39.18	8
ATOM	4035	OW1	WAT	X	14	16.344	4.264	16.031	1.00	22.00	8
ATOM	4036	OW2	WAT	X	14	32.347	13.546	-3.049	1.00	37.27	8
ATOM	4037	OW3	WAT	X	14	45.366	38.058	33.758	1.00	20.90	8
ATOM	4038	OW4	WAT	X	14	4.549	18.600	13.099	1.00	20.30	8
ATOM	4039	OW5	WAT	X	14	15.354	36.796	43.569	1.00	18.79	8
ATOM	4040	OW6	WAT	X	14	44.963	30.462	57.791	1.00	33.45	8
ATOM	4041	OW7	WAT	X	14	53.136	23.195	37.475	1.00	31.43	8
ATOM	4042	OW8	WAT	X	14	30.694	15.659	-3.842	1.00	23.59	8
ATOM	4043	OW9	WAT	X	14	39.010	7.257	14.525	1.00	37.98	8
ATOM	4044	OW0	WAT	X	15	37.498	55.360	32.899	1.00	35.04	8
ATOM	4045	OW1	WAT	X	15	21.133	44.448	35.481	1.00	35.84	8
ATOM	4046	OW2	WAT	X	15	23.993	4.153	14.519	1.00	20.07	8
ATOM	4047	OW3	WAT	X	15	21.568	23.231	44.662	1.00	34.60	8
ATOM	4048	OW4	WAT	X	15	9.185	24.466	6.708	1.00	19.79	8
ATOM	4049	OW5	WAT	X	15	44.586	35.812	31.349	1.00	48.30	8
ATOM	4050	OW6	WAT	X	15	30.789	25.745	52.371	1.00	38.63	8
ATOM	4051	OW7	WAT	X	15	41.284	38.972	11.403	1.00	29.22	8
ATOM	4052	OW8	WAT	X	15	56.979	36.187	58.016	1.00	37.19	8
ATOM	4053	OW9	WAT	X	15	25.886	5.827	3.524	1.00	21.64	8
ATOM	4054	OW0	WAT	X	16	41.689	14.341	39.346	1.00	28.91	8
ATOM	4055	OW1	WAT	X	16	20.238	10.905	31.899	1.00	29.69	8
ATOM	4056	OW2	WAT	X	16	44.542	44.756	52.978	1.00	18.83	8
ATOM	4057	OW3	WAT	X	16	57.377	17.228	51.604	1.00	20.62	8
ATOM	4058	OW4	WAT	X	16	53.851	33.580	56.957	1.00	22.46	8
ATOM	4059	OW5	WAT	X	16	35.776	25.007	52.963	1.00	30.96	8
ATOM	4060	OW6	WAT	X	16	50.697	26.378	37.894	1.00	17.69	8
ATOM	4061	OW7	WAT	X	16	35.244	16.237	47.346	1.00	35.92	8
ATOM	4062	OW8	WAT	X	16	41.297	31.972	30.043	1.00	23.15	8
ATOM	4063	OW9	WAT	X	16	60.104	21.780	53.887	1.00	24.69	8
ATOM	4064	OW0	WAT	X	17	33.930	36.911	56.317	1.00	28.54	8
ATOM	4065	OW1	WAT	X	17	27.783	49.620	50.985	1.00	21.73	8
ATOM	4066	OW2	WAT	X	17	38.322	12.309	23.483	1.00	42.93	8
ATOM	4067	OW3	WAT	X	17	19.759	16.587	26.896	1.00	25.91	8
ATOM	4068	OW4	WAT	X	17	18.392	24.561	-0.866	1.00	45.44	8
ATOM	4069	OW5	WAT	X	17	43.370	16.553	29.268	1.00	24.28	8
ATOM	4070	OW6	WAT	X	17	12.508	25.520	4.810	1.00	39.21	8
ATOM	4071	OW7	WAT	X	17	44.009	35.484	9.586	1.00	24.72	8
ATOM	4072	OW8	WAT	X	17	38.155	15.958	4.049	1.00	27.73	8
ATOM	4073	OW9	WAT	X	17	32.659	22.367	51.695	1.00	36.96	8
ATOM	4074	OW0	WAT	X	18	8.655	11.822	18.551	1.00	22.83	8
ATOM	4075	OW1	WAT	X	18	61.442	16.332	49.671	1.00	35.09	8
ATOM	4076	OW2	WAT	X	18	52.691	20.468	49.830	1.00	27.27	8
ATOM	4077	OW3	WAT	X	18	33.981	29.452	4.620	1.00	46.70	8
ATOM	4078	OW4	WAT	X	18	22.398	9.094	32.744	1.00	31.90	8
ATOM	4079	OW5	WAT	X	18	24.654	27.519	4.442	1.00	26.37	8
ATOM	4080	OW6	WAT	X	18	24.112	52.226	27.595	1.00	38.43	8
ATOM	4081	OW7	WAT	X	18	33.663	55.271	29.435	1.00	43.20	8
ATOM	4082	OW8	WAT	X	18	30.748	53.658	50.670	1.00	29.38	8
ATOM	4083	OW9	WAT	X	18	50.065	24.808	35.502	1.00	35.76	8
ATOM	4084	OW0	WAT	X	19	22.202	19.032	28.774	1.00	27.27	8
ATOM	4085	OW1	WAT	X	19	54.614	46.941	48.285	1.00	29.46	8
ATOM	4086	OW2	WAT	X	19	46.049	21.147	25.386	1.00	53.35	8
ATOM	4087	OW3	WAT	X	19	45.816	49.038	43.196	1.00	33.55	8
ATOM	4088	OW4	WAT	X	19	22.659	43.614	47.560	1.00	46.32	8
ATOM	4089	OW5	WAT	X	19	60.822	30.153	59.870	1.00	43.42	8
ATOM	4090	OW6	WAT	X	19	53.393	13.840	38.545	1.00	34.26	8
ATOM	4091	OW7	WAT	X	19	32.544	1.677	6.989	1.00	38.69	8
ATOM	4092	OW8	WAT	X	19	50.647	31.408	63.808	1.00	33.78	8
ATOM	4093	OW9	WAT	X	19	16.948	27.505	19.812	1.00	23.95	8
ATOM	4094	OW0	WAT	X	20	6.330	5.129	-1.860	1.00	55.10	8
ATOM	4095	OW1	WAT	X	20	32.149	29.484	1.396	1.00	29.24	8
ATOM	4096	OW2	WAT	X	20	18.952	20.628	24.894	1.00	35.86	8
ATOM	4097	OW3	WAT	X	20	31.733	56.172	34.803	1.00	38.99	8
ATOM	4098	OW4	WAT	X	20	54.293	14.452	50.415	1.00	35.67	8
ATOM	4099	OW5	WAT	X	20	44.169	20.632	26.756	1.00	27.57	8
ATOM	4100	OW6	WAT	X	20	25.114	53.998	30.655	1.00	43.33	8
ATOM	4101	OW7	WAT	X	20	43.966	46.309	55.136	1.00	37.54	8
ATOM	4102	OW8	WAT	X	20	58.366	45.019	48.175	1.00	43.14	8
ATOM	4103	OW9	WAT	X	20	44.205	21.201	13.125	1.00	51.53	8
ATOM	4104	OW0	WAT	X	21	61.128	25.016	42.919	1.00	34.86	8
ATOM	4105	OW1	WAT	X	21	8.371	24.444	12.113	1.00	45.95	8
ATOM	4106	OW2	WAT	X	21	18.370	31.505	12.739	1.00	27.20	8
ATOM	4107	OW3	WAT	X	21	33.430	25.045	51.739	1.00	31.92	8
ATOM	4108	OW4	WAT	X	21	47.660	31.418	59.018	1.00	35.64	8
ATOM	4109	OW5	WAT	X	21	43.308	25.115	12.609	1.00	40.37	8
ATOM	4110	OW6	WAT	X	21	44.725	50.787	28.523	1.00	26.83	8
ATOM	4111	OW7	WAT	X	21	40.073	41.591	56.477	1.00	38.23	8
ATOM	4112	OW8	WAT	X	21	3.706	15.718	9.641	1.00	23.55	8
ATOM	4113	OW9	WAT	X	21	46.527	18.879	50.827	1.00	35.55	8
ATOM	4114	OW0	WAT	X	22	51.052	12.865	45.163	1.00	48.72	8
ATOM	4115	OW1	WAT	X	22	54.191	42.505	55.913	1.00	22.39	8
ATOM	4116	OW2	WAT	X	22	65.480	31.263	47.436	1.00	36.62	8
ATOM	4117	OW3	WAT	X	22	30.283	47.935	54.169	1.00	31.71	8
ATOM	4118	OW4	WAT	X	22	35.283	36.318	46.899	1.00	68.71	8
ATOM	4119	OW5	WAT	X	22	47.871	46.056	38.969	1.00	32.78	8
ATOM	4120	OW6	WAT	X	22	37.896	8.826	3.495	1.00	35.54	8
ATOM	4121	OW7	WAT	X	22	35.101	8.628	38.130	1.00	35.44	8
ATOM	4122	OW8	WAT	X	22	38.308	4.945	9.263	1.00	39.44	8
ATOM	4123	OW9	WAT	X	22	29.192	42.186	18.601	1.00	35.54	8
ATOM	4124	OW0	WAT	X	23	43.449	25.207	33.605	1.00	42.65	8
ATOM	4125	OW1	WAT	X	23	42.056	26.583	57.914	1.00	44.04	8
ATOM	4126	OW2	WAT	X	23	15.436	32.096	27.975	1.00	29.94	8
ATOM	4127	OW3	WAT	X	23	40.123	43.268	18.152	1.00	37.43	8
ATOM	4128	OW4	WAT	X	23	14.301	18.529	21.331	1.00	32.32	8
ATOM	4129	OW5	WAT	X	23	41.316	39.786	58.213	1.00	42.06	8
ATOM	4130	OW6	WAT	X	23	28.167	15.941	46.987	1.00	39.62	8
ATOM	4131	OW7	WAT	X	23	62.463	32.861	38.118	1.00	33.05	8
ATOM	4132	OW8	WAT	X	23	50.420	44.042	41.952	1.00	24.23	8
ATOM	4133	OW9	WAT	X	23	30.486	6.686	18.716	1.00	37.32	8
ATOM	4134	OW0	WAT	X	24	39.000	11.315	44.273	1.00	38.40	8

ATOM	4135	OW1	WAT	X	24	26.342	44.842	18.030	1.00	27.39	8
ATOM	4136	OW2	WAT	X	24	42.233	42.967	22.516	1.00	28.16	8
ATOM	4137	OW3	WAT	X	24	17.859	41.857	40.950	1.00	44.87	8
ATOM	4138	OW4	WAT	X	24	18.774	45.302	34.094	1.00	36.85	8
ATOM	4139	OW5	WAT	X	24	17.379	48.385	29.218	1.00	36.40	8
ATOM	4140	OW6	WAT	X	24	59.859	17.628	38.947	1.00	24.00	8
ATOM	4141	OW7	WAT	X	24	44.716	26.845	15.361	1.00	31.66	8
ATOM	4142	OW8	WAT	X	24	16.851	22.367	25.144	1.00	38.33	8
ATOM	4143	OW9	WAT	X	24	44.428	18.344	31.454	1.00	28.87	8
ATOM	4144	OW0	WAT	X	25	53.824	36.690	57.769	1.00	27.33	8
ATOM	4145	OW1	WAT	X	25	53.688	40.328	57.339	1.00	34.91	8
ATOM	4146	OW2	WAT	X	25	46.373	15.118	12.832	1.00	38.80	8
ATOM	4147	OW3	WAT	X	25	29.409	35.711	7.581	1.00	30.09	8
ATOM	4148	OW4	WAT	X	25	26.515	13.237	-3.213	1.00	30.52	8
ATOM	4149	OW5	WAT	X	25	20.273	3.147	6.130	1.00	29.22	8
ATOM	4150	OW6	WAT	X	25	34.514	42.011	19.633	1.00	23.60	8
ATOM	4151	OW7	WAT	X	25	41.463	52.238	24.622	1.00	33.83	8
ATOM	4152	OW8	WAT	X	25	18.346	37.804	42.302	1.00	35.93	8
ATOM	4153	OW9	WAT	X	25	35.262	54.671	32.179	1.00	58.94	8
ATOM	4154	OW0	WAT	X	26	44.229	16.673	16.585	1.00	37.25	8
ATOM	4155	OW1	WAT	X	26	44.766	14.121	14.699	1.00	46.53	8
ATOM	4156	OW2	WAT	X	26	31.390	33.920	59.134	1.00	33.03	8
ATOM	4157	OW3	WAT	X	26	12.971	21.397	23.449	1.00	37.99	8
ATOM	4158	OW4	WAT	X	26	41.259	51.310	51.509	1.00	40.81	8
ATOM	4159	OW5	WAT	X	26	41.929	11.622	42.697	1.00	45.17	8
ATOM	4160	OW6	WAT	X	26	42.707	44.751	57.570	1.00	42.32	8
ATOM	4161	OW7	WAT	X	26	56.463	43.749	51.681	1.00	36.66	8
ATOM	4162	OW8	WAT	X	26	24.821	11.342	-3.728	1.00	33.27	8
ATOM	4163	OW9	WAT	X	26	60.493	39.175	53.713	1.00	47.98	8
ATOM	4164	OW0	WAT	X	27	45.625	38.306	11.910	1.00	37.28	8
ATOM	4165	OW1	WAT	X	27	43.801	49.874	24.898	1.00	75.50	8
ATOM	4166	OW2	WAT	X	27	11.684	17.068	21.179	1.00	34.01	8
ATOM	4167	OW3	WAT	X	27	28.216	2.149	14.807	1.00	42.07	8
ATOM	4168	OW4	WAT	X	27	52.604	30.867	37.880	1.00	33.10	8
ATOM	4169	OW5	WAT	X	27	55.458	34.651	38.180	1.00	47.45	8
ATOM	4170	OW6	WAT	X	27	49.808	19.847	34.189	1.00	33.89	8
ATOM	4171	OW7	WAT	X	27	1.703	6.632	4.199	1.00	62.88	8
ATOM	4172	OW8	WAT	X	27	48.275	39.555	43.586	1.00	28.38	8
ATOM	4173	OW9	WAT	X	27	23.075	20.226	-6.003	1.00	61.62	8
ATOM	4174	OW0	WAT	X	28	38.679	43.247	57.111	1.00	53.07	8
ATOM	4175	OW1	WAT	X	28	21.533	51.639	33.545	1.00	49.86	8
ATOM	4176	OW2	WAT	X	28	1.544	11.851	5.024	1.00	69.29	8
ATOM	4177	OW3	WAT	X	28	22.566	43.229	15.525	1.00	28.33	8
ATOM	4178	OW4	WAT	X	28	44.851	57.241	34.859	1.00	42.49	8
ATOM	4179	OW5	WAT	X	28	33.378	9.541	42.581	1.00	51.22	8
ATOM	4180	OW6	WAT	X	28	27.186	6.024	-0.021	1.00	46.35	8
ATOM	4181	OW7	WAT	X	28	56.162	41.254	59.120	1.00	56.59	8
ATOM	4182	OW8	WAT	X	28	5.756	19.201	7.132	1.00	20.05	8
ATOM	4183	OW9	WAT	X	28	14.700	29.886	48.605	1.00	35.67	8
ATOM	4184	OW0	WAT	X	29	41.585	56.275	32.373	1.00	42.13	8
ATOM	4185	OW1	WAT	X	29	24.084	49.694	43.922	1.00	40.12	8
ATOM	4186	OW2	WAT	X	29	29.979	22.421	2.045	1.00	42.88	8
ATOM	4187	OW3	WAT	X	29	18.885	13.752	26.566	1.00	49.31	8
ATOM	4188	OW4	WAT	X	29	33.246	35.860	58.555	1.00	24.66	8
ATOM	4189	OW5	WAT	X	29	20.518	10.712	22.033	1.00	31.01	8
ATOM	4190	OW6	WAT	X	29	28.355	41.870	50.614	1.00	38.09	8
ATOM	4191	OW7	WAT	X	29	51.144	33.741	38.200	1.00	28.11	8
ATOM	4192	OW8	WAT	X	29	50.909	32.604	61.158	1.00	44.30	8
ATOM	4193	OW9	WAT	X	29	45.397	9.987	33.816	1.00	41.23	8
ATOM	4194	OW0	WAT	X	30	45.383	21.851	32.647	1.00	34.24	8
ATOM	4195	OW1	WAT	X	30	51.981	22.543	34.910	1.00	43.50	8
ATOM	4196	OW2	WAT	X	30	35.294	58.821	39.452	1.00	34.28	8
ATOM	4197	OW3	WAT	X	30	34.193	44.616	18.067	1.00	42.78	8
ATOM	4198	OW4	WAT	X	30	31.695	52.889	53.190	1.00	54.83	8
ATOM	4199	OW5	WAT	X	30	13.657	44.210	31.115	1.00	42.94	8
ATOM	4200	OW6	WAT	X	30	17.493	40.635	13.227	1.00	54.30	8
ATOM	4201	OW7	WAT	X	30	24.521	11.373	22.566	1.00	42.89	8
ATOM	4202	OW8	WAT	X	30	37.671	38.607	58.700	1.00	67.82	8
ATOM	4203	OW9	WAT	X	30	8.539	26.332	10.421	1.00	56.80	8
ATOM	4204	OW0	WAT	X	31	49.681	16.792	34.456	1.00	56.81	8
ATOM	4205	OW1	WAT	X	31	7.284	6.777	13.925	1.00	41.62	8
ATOM	4206	OW2	WAT	X	31	19.842	44.869	37.796	1.00	32.48	8
ATOM	4207	OW3	WAT	X	31	16.806	43.159	34.050	1.00	31.63	8
ATOM	4208	OW4	WAT	X	31	40.080	55.247	29.931	1.00	46.41	8
ATOM	4209	OW5	WAT	X	31	4.298	25.496	15.931	1.00	55.22	8
ATOM	4210	OW6	WAT	X	31	49.649	40.424	40.847	1.00	31.66	8
ATOM	4211	OW7	WAT	X	31	22.128	29.127	52.419	1.00	40.80	8
ATOM	4212	OW8	WAT	X	31	16.243	33.605	36.184	1.00	38.09	8
ATOM	4213	OW9	WAT	X	31	27.033	55.215	28.323	1.00	31.92	8
ATOM	4214	OW0	WAT	X	32	16.931	37.637	36.501	1.00	32.22	8
ATOM	4215	OW1	WAT	X	32	7.050	10.385	16.890	1.00	37.40	8
ATOM	4216	OW2	WAT	X	32	50.382	29.410	35.312	1.00	56.52	8
ATOM	4217	OW3	WAT	X	32	27.086	47.626	17.616	1.00	31.50	8
ATOM	4218	OW4	WAT	X	32	50.029	47.652	42.125	1.00	45.87	8
ATOM	4219	OW5	WAT	X	32	29.154	55.495	24.292	1.00	53.90	8
ATOM	4220	OW6	WAT	X	32	32.970	58.606	36.552	1.00	46.22	8
ATOM	4221	OW7	WAT	X	32	43.201	24.152	56.971	1.00	59.17	8
ATOM	4222	OW8	WAT	X	32	41.947	30.732	9.284	1.00	45.99	8
ATOM	4223	OW9	WAT	X	32	21.381	14.261	36.815	1.00	44.69	8
ATOM	4224	OW0	WAT	X	33	60.941	22.089	43.042	1.00	37.06	8
ATOM	4225	OW1	WAT	X	33	40.505	56.155	42.947	1.00	68.99	8
ATOM	4226	OW3	WAT	X	33	18.578	37.434	47.553	1.00	35.06	8
ATOM	4227	OW4	WAT	X	33	31.707	48.490	18.182	1.00	32.40	8
ATOM	4228	OW5	WAT	X	33	20.611	21.237	38.626	1.00	41.44	8
ATOM	4229	OW6	WAT	X	33	38.037	8.708	21.690	1.00	53.54	8
ATOM	4230	OW7	WAT	X	33	18.925	37.694	11.766	1.00	57.07	8
ATOM	4231	OW8	WAT	X	33	53.097	28.032	37.987	1.00	57.12	8
ATOM	4232	OW9	WAT	X	33	63.148	36.349	37.733	1.00	40.38	8
ATOM	4233	OW0	WAT	X	34	14.116	36.171	21.843	1.00	42.46	8
ATOM	4234	OW1	WAT	X	34	22.608	32.412	5.553	1.00	37.92	8
ATOM	4235	OW2	WAT	X	34	29.443	3.779	16.367	1.00	46.74	8
ATOM	4236	OW3	WAT	X	34	41.862	17.565	7.880	1.00	10.16	8
ATOM	4237	OW4	WAT	X	34	44.558	18.412	8.333	1.00	38.61	8
ATOM	4238	OW5	WAT	X	34	51.913	26.058	58.542	1.00	43.05	8
ATOM	4239	OW6	WAT	X	34	64.063	33.656	56.634	1.00	55.33	8
ATOM	4240	OW7	WAT	X	34	34.660	53.702	52.276	1.00	47.20	8

ATOM	4241	OW8	WAT	X	34	5.844	14.713	12.911	1.00	40.12	8
ATOM	4242	OW9	WAT	X	34	39.697	54.257	50.395	1.00	36.68	8
ATOM	4243	OW0	WAT	X	35	18.706	24.537	40.234	1.00	51.89	8
ATOM	4244	OW1	WAT	X	35	20.209	21.570	34.426	1.00	34.23	8
ATOM	4245	OW2	WAT	X	35	44.584	17.646	26.801	1.00	35.48	8
ATOM	4246	OW3	WAT	X	35	61.438	32.246	57.799	1.00	36.05	8
ATOM	4247	OW4	WAT	X	35	13.266	6.166	0.033	1.00	49.60	8
ATOM	4248	OW5	WAT	X	35	42.142	53.175	26.887	1.00	43.15	8
ATOM	4249	OW6	WAT	X	35	33.505	54.214	55.522	1.00	56.63	8
ATOM	4250	OW7	WAT	X	35	1.397	8.422	6.873	1.00	48.68	8
ATOM	4251	OW8	WAT	X	35	47.778	11.907	38.953	1.00	34.48	8
ATOM	4252	OW9	WAT	X	35	15.856	27.767	43.603	1.00	55.40	8
ATOM	4253	OW0	WAT	X	36	38.734	7.626	16.829	1.00	43.46	8
ATOM	4254	OW1	WAT	X	36	10.578	1.626	2.281	1.00	40.52	8
ATOM	4255	OW2	WAT	X	36	50.000	33.901	35.051	1.00	49.14	8
ATOM	4256	OW3	WAT	X	36	44.622	34.879	33.356	1.00	60.84	8
ATOM	4257	OW4	WAT	X	36	3.016	16.327	21.655	1.00	60.04	8
ATOM	4258	OW5	WAT	X	36	41.431	56.503	45.767	1.00	56.22	8
ATOM	4259	OW6	WAT	X	36	49.548	26.337	22.216	1.00	53.09	8
ATOM	4260	OW7	WAT	X	36	37.549	29.346	4.956	1.00	52.92	8
ATOM	4261	OW8	WAT	X	36	49.240	44.486	55.149	1.00	38.00	8
ATOM	4262	OW9	WAT	X	36	53.734	18.532	52.401	1.00	51.95	8
ATOM	4263	OW0	WAT	X	37	39.041	11.166	25.898	1.00	36.59	8
ATOM	4264	OW1	WAT	X	37	10.532	4.916	16.271	1.00	58.74	8
ATOM	4265	OW2	WAT	X	37	41.346	7.373	32.768	1.00	47.04	8
ATOM	4266	OW3	WAT	X	37	32.474	41.914	15.484	1.00	44.27	8
ATOM	4267	OW4	WAT	X	37	18.592	28.534	17.648	1.00	41.36	8
ATOM	4268	OW5	WAT	X	37	58.677	25.814	40.128	1.00	40.22	8
ATOM	4269	OW6	WAT	X	37	15.547	6.537	19.083	1.00	45.33	8
ATOM	4270	OW7	WAT	X	37	37.675	57.053	47.412	1.00	49.88	8
ATOM	4271	OW8	WAT	X	37	49.434	37.594	42.185	1.00	39.96	8
ATOM	4272	OW9	WAT	X	37	42.690	28.862	30.545	1.00	42.38	8
ATOM	4273	OW0	WAT	X	38	29.822	6.331	24.708	1.00	48.41	8
ATOM	4274	OW2	WAT	X	38	43.889	32.981	31.239	1.00	43.26	8
ATOM	4275	OW3	WAT	X	38	16.119	10.852	-3.221	1.00	36.08	8
ATOM	4276	OW4	WAT	X	38	46.051	14.381	33.005	1.00	54.04	8
ATOM	4277	OW5	WAT	X	38	26.231	44.941	50.291	1.00	58.57	8
ATOM	4278	OW6	WAT	X	38	41.500	26.375	9.990	1.00	50.76	8
ATOM	4279	OW7	WAT	X	38	51.550	42.087	41.209	1.00	49.03	8
ATOM	4280	OW8	WAT	X	38	38.215	7.892	30.920	1.00	52.61	8
ATOM	4281	OW9	WAT	X	38	22.207	33.878	7.842	1.00	43.87	8
ATOM	4282	OW0	WAT	X	39	49.722	41.667	12.969	1.00	47.74	8
ATOM	4283	OW1	WAT	X	39	35.909	18.255	51.330	1.00	59.07	8
ATOM	4284	OW2	WAT	X	39	43.924	10.373	31.316	1.00	53.37	8
ATOM	4285	OW3	WAT	X	39	22.583	10.397	39.495	1.00	42.79	8
ATOM	4286	OW4	WAT	X	39	19.514	48.906	21.847	1.00	68.43	8
ATOM	4287	OW5	WAT	X	39	13.468	27.723	5.713	1.00	66.89	8
ATOM	4288	OW6	WAT	X	39	45.654	25.542	63.943	1.00	44.03	8
ATOM	4289	OW7	WAT	X	39	44.078	13.029	36.046	1.00	37.57	8
ATOM	4290	OW8	WAT	X	39	27.240	0.087	12.290	1.00	48.13	8
ATOM	4291	OW9	WAT	X	39	15.804	17.374	23.289	1.00	45.09	8
ATOM	4292	OW0	WAT	X	40	23.294	12.036	34.534	1.00	58.48	8
ATOM	4293	OW1	WAT	X	40	47.490	44.003	18.065	1.00	60.75	8
ATOM	4294	OW2	WAT	X	40	17.196	19.679	22.860	1.00	53.81	8
ATOM	4295	OW3	WAT	X	40	22.069	3.918	3.047	1.00	55.02	8
ATOM	4296	OW4	WAT	X	40	40.725	28.659	11.393	1.00	42.24	8
ATOM	4297	OW5	WAT	X	40	53.521	31.821	60.008	1.00	46.58	8
ATOM	4298	OW6	WAT	X	40	43.778	45.011	23.792	1.00	52.91	8
ATOM	4299	OW7	WAT	X	40	45.725	48.904	30.294	1.00	35.75	8
ATOM	4300	OW8	WAT	X	40	49.126	11.559	46.679	1.00	49.02	8
ATOM	4301	OW9	WAT	X	40	68.137	39.801	42.467	1.00	64.82	8
ATOM	4302	OW0	WAT	X	41	19.785	19.132	28.386	1.00	38.16	8
ATOM	4303	OW1	WAT	X	41	46.799	34.048	27.779	1.00	53.88	8
ATOM	4304	OW2	WAT	X	41	46.195	38.407	29.718	1.00	67.17	8
ATOM	4305	OW3	WAT	X	41	10.791	46.608	27.796	1.00	38.46	8
ATOM	4306	OW4	WAT	X	41	17.255	25.962	28.182	1.00	49.71	8
ATOM	4307	OW5	WAT	X	41	38.815	10.903	18.927	1.00	49.73	8
ATOM	4308	OW6	WAT	X	41	47.017	51.069	47.161	1.00	58.10	8
ATOM	4309	OW7	WAT	X	41	52.558	36.860	39.163	1.00	53.80	8
ATOM	4310	OW8	WAT	X	41	19.024	23.922	31.261	1.00	60.30	8
ATOM	4311	OW9	WAT	X	41	15.798	27.427	30.407	1.00	100.00	8
ATOM	4312	OW0	WAT	X	42	55.428	38.709	38.776	1.00	50.63	8
ATOM	4313	OW1	WAT	X	42	23.391	20.916	45.890	1.00	44.61	8
ATOM	4314	OW2	WAT	X	42	4.072	14.391	18.394	1.00	42.40	8
ATOM	4315	OW3	WAT	X	42	42.371	37.835	9.565	1.00	46.80	8
ATOM	4316	OW4	WAT	X	42	6.020	13.143	15.676	1.00	60.89	8
ATOM	4317	OW5	WAT	X	42	2.445	17.737	5.335	1.00	44.54	8
ATOM	4318	OW6	WAT	X	42	39.431	8.272	34.812	1.00	46.23	8
ATOM	4319	OW7	WAT	X	42	43.239	42.762	20.441	1.00	42.07	8
ATOM	4320	OW8	WAT	X	42	43.667	29.029	33.074	1.00	53.81	8
ATOM	4321	OW9	WAT	X	42	15.819	3.536	11.715	1.00	45.41	8
ATOM	4322	OW0	WAT	X	43	22.756	6.724	-4.904	1.00	44.46	8
ATOM	4323	OW1	WAT	X	43	32.918	47.694	61.485	1.00	67.38	8
ATOM	4324	OW2	WAT	X	43	32.074	40.098	11.945	1.00	34.37	8
ATOM	4325	OW3	WAT	X	43	44.790	41.553	18.449	1.00	44.94	8
ATOM	4326	OW4	WAT	X	43	15.058	29.090	20.720	1.00	49.25	8
ATOM	4327	OW5	WAT	X	43	24.069	18.351	48.150	1.00	62.06	8
ATOM	4328	OW6	WAT	X	43	40.835	26.920	30.843	1.00	49.68	8
ATOM	4329	OW7	WAT	X	43	7.082	2.097	8.379	1.00	47.50	8
ATOM	4330	OW8	WAT	X	43	47.039	51.990	40.775	1.00	51.23	8
ATOM	4331	OW9	WAT	X	43	22.252	13.968	43.293	1.00	38.13	8
ATOM	4332	OW0	WAT	X	44	25.106	31.488	52.711	1.00	57.06	8
ATOM	4333	OW1	WAT	X	44	23.054	7.691	28.407	1.00	52.15	8
ATOM	4334	OW2	WAT	X	44	21.526	1.631	11.156	1.00	53.95	8
ATOM	4335	OW3	WAT	X	44	20.140	16.123	39.073	1.00	62.86	8
ATOM	4336	OW4	WAT	X	44	17.491	51.997	31.031	1.00	80.00	8
ATOM	4337	OW5	WAT	X	44	46.380	42.021	59.675	1.00	51.50	8
ATOM	4338	OW6	WAT	X	44	13.481	34.188	29.544	1.00	66.53	8
ATOM	4339	OW7	WAT	X	44	33.452	41.508	56.803	1.00	50.62	8
ATOM	4340	OW8	WAT	X	44	47.624	43.632	31.945	1.00	43.18	8
ATOM	4341	OW9	WAT	X	44	26.231	12.181	43.880	1.00	49.95	8
ATOM	4342	OW0	WAT	X	45	14.968	36.024	33.676	1.00	63.17	8
ATOM	4343	OW1	WAT	X	45	62.906	20.054	42.528	1.00	50.37	8
ATOM	4344	OW2	WAT	X	45	45.852	21.374	58.053	1.00	55.98	8
ATOM	4345	OW3	WAT	X	45	50.504	43.538	16.798	1.00	34.36	8
ATOM	4346	OW4	WAT	X	45	36.077	40.800	13.082	1.00	45.23	8

ATOM	4347	OW5	WAT	X	45	15.297	36.178	30.314	1.00	41.94	8
ATOM	4348	OW6	WAT	X	45	11.948	34.622	19.560	1.00	83.16	8
ATOM	4349	OW8	WAT	X	45	49.746	24.887	60.391	1.00	66.28	8
ATOM	4350	OW9	WAT	X	45	36.657	55.115	28.131	1.00	37.69	8
ATOM	4351	OW0	WAT	X	46	55.074	25.248	36.950	1.00	41.36	8
ATOM	4352	OW1	WAT	X	46	47.652	23.423	22.484	1.00	42.59	8
ATOM	4353	OW2	WAT	X	46	44.015	15.772	24.447	1.00	47.57	8
ATOM	4354	OW3	WAT	X	46	7.635	2.279	10.856	1.00	61.51	8
ATOM	4355	OW4	WAT	X	46	55.490	45.238	53.756	1.00	80.18	8
ATOM	4356	OW5	WAT	X	46	24.651	30.369	3.824	1.00	53.51	8
ATOM	4357	OW6	WAT	X	46	36.564	25.795	58.795	1.00	43.24	8
ATOM	4358	OW7	WAT	X	46	37.878	24.510	56.673	1.00	60.23	8
ATOM	4359	OW8	WAT	X	46	9.767	27.253	17.228	1.00	44.01	8
ATOM	4360	OW9	WAT	X	46	33.066	7.229	37.529	1.00	48.47	8
ATOM	4361	OW0	WAT	X	47	8.243	21.706	21.929	1.00	61.56	8
ATOM	4362	OW1	WAT	X	47	46.978	13.274	45.175	1.00	40.90	8
ATOM	4363	OW2	WAT	X	47	41.004	12.753	21.561	1.00	73.88	8
ATOM	4364	OW4	WAT	X	47	3.035	8.918	-0.355	1.00	50.88	8
ATOM	4365	OW5	WAT	X	47	18.537	34.248	10.555	1.00	79.91	8
ATOM	4366	OW6	WAT	X	47	26.233	6.791	-2.079	1.00	48.58	8
ATOM	4367	OW7	WAT	X	47	37.312	53.735	22.566	1.00	63.31	8
ATOM	4368	OW8	WAT	X	47	17.940	29.638	6.277	1.00	57.32	8
ATOM	4369	OW9	WAT	X	47	26.830	27.316	2.717	1.00	62.15	8
ATOM	4370	OW0	WAT	X	48	65.931	28.577	46.176	1.00	69.51	8
ATOM	4371	OW1	WAT	X	48	19.661	45.120	40.540	1.00	40.74	8
ATOM	4372	OW2	WAT	X	48	10.667	22.744	23.628	1.00	36.22	8
ATOM	4373	OW3	WAT	X	48	8.702	24.434	20.838	1.00	51.66	8
ATOM	4374	OW4	WAT	X	48	35.773	26.533	56.343	1.00	38.96	8
ATOM	4375	OW5	WAT	X	48	38.218	2.333	13.072	1.00	37.60	8
ATOM	4376	OW6	WAT	X	48	25.061	48.128	50.748	1.00	69.43	8
ATOM	4377	OW7	WAT	X	48	24.333	37.538	52.402	1.00	33.69	8
ATOM	4378	OW8	WAT	X	48	52.741	13.029	46.552	1.00	46.94	8
ATOM	4379	OW9	WAT	X	48	30.393	18.085	52.715	1.00	73.77	8
ATOM	4380	OW0	WAT	X	49	21.293	35.987	52.496	1.00	56.71	8
ATOM	4381	OW1	WAT	X	49	26.704	53.743	20.826	1.00	82.73	8
ATOM	4382	OW2	WAT	X	49	65.451	38.921	50.670	1.00	50.91	8
ATOM	4383	OW3	WAT	X	49	9.019	18.103	21.967	1.00	57.54	8
ATOM	4384	OW4	WAT	X	49	43.689	31.759	26.580	1.00	33.20	8
ATOM	4385	OW5	WAT	X	49	65.973	31.154	38.950	1.00	51.21	8
ATOM	4386	OW6	WAT	X	49	50.668	41.968	57.102	1.00	65.20	8
ATOM	4387	OW7	WAT	X	49	67.466	32.818	48.733	1.00	35.55	8
ATOM	4388	OW8	WAT	X	49	12.540	31.451	14.136	1.00	67.07	8
ATOM	4389	OW9	WAT	X	49	24.089	6.493	18.874	1.00	41.89	8
ATOM	4390	OW0	WAT	X	50	46.352	12.360	48.271	1.00	78.91	8
ATOM	4391	OW1	WAT	X	50	26.960	36.851	6.038	1.00	44.57	8
ATOM	4392	OW2	WAT	X	50	37.082	59.754	36.774	1.00	66.16	8
ATOM	4393	OW3	WAT	X	50	57.220	36.380	35.486	1.00	60.08	8
ATOM	4394	OW4	WAT	X	50	47.460	48.140	35.950	1.00	51.89	8
ATOM	4395	OW5	WAT	X	50	32.642	7.671	29.024	1.00	62.58	8
ATOM	4396	OW6	WAT	X	50	40.898	5.278	12.690	1.00	58.65	8
ATOM	4397	OW7	WAT	X	50	43.951	11.795	23.808	1.00	51.02	8
ATOM	4398	OW8	WAT	X	50	56.331	38.665	59.400	1.00	77.23	8
ATOM	4399	OW9	WAT	X	50	42.112	15.859	19.271	1.00	42.44	8
ATOM	4400	OW0	WAT	X	51	43.751	9.508	10.207	1.00	72.09	8
ATOM	4401	OW1	WAT	X	51	21.156	18.175	-5.366	1.00	59.15	8
ATOM	4402	OW2	WAT	X	51	20.822	20.591	30.625	1.00	53.15	8
ATOM	4403	OW3	WAT	X	51	25.847	41.728	50.223	1.00	53.16	8
ATOM	4404	OW4	WAT	X	51	42.406	49.560	54.444	1.00	49.42	8
ATOM	4405	OW5	WAT	X	51	11.152	-0.096	4.529	1.00	73.12	8
ATOM	4406	OW6	WAT	X	51	41.064	10.519	39.198	1.00	76.33	8
ATOM	4407	OW7	WAT	X	51	11.838	45.652	24.174	1.00	52.20	8
ATOM	4408	OW8	WAT	X	51	24.803	8.502	38.134	1.00	48.46	8
ATOM	4409	OW9	WAT	X	51	28.241	55.029	32.933	1.00	56.81	8
ATOM	4410	OW0	WAT	X	52	24.326	46.042	48.362	1.00	42.89	8
ATOM	4411	OW1	WAT	X	52	60.372	23.243	57.581	1.00	51.46	8
ATOM	4412	OW2	WAT	X	52	44.063	13.149	3.195	1.00	73.23	8
ATOM	4413	OW3	WAT	X	52	29.959	38.273	7.993	1.00	74.96	8
ATOM	4414	OW4	WAT	X	52	17.959	47.341	32.823	1.00	52.58	8
ATOM	4415	OW5	WAT	X	52	35.761	36.887	7.808	1.00	46.76	8
ATOM	4416	OW6	WAT	X	52	29.185	14.140	50.554	1.00	100.00	8
ATOM	4417	OW7	WAT	X	52	46.852	47.409	54.235	1.00	47.47	8
ATOM	4418	OW8	WAT	X	52	46.124	18.871	10.000	1.00	74.45	8
ATOM	4419	OW9	WAT	X	52	43.467	42.127	14.225	1.00	58.70	8
ATOM	4420	OW1	WAT	X	53	42.354	10.824	26.570	1.00	74.16	8
ATOM	4421	OW2	WAT	X	53	41.382	9.160	28.416	1.00	65.06	8
ATOM	4422	OW3	WAT	X	53	32.249	16.276	51.085	1.00	66.53	8
ATOM	4423	OW4	WAT	X	53	43.754	20.935	55.297	1.00	89.21	8
ATOM	4424	OW5	WAT	X	53	46.525	22.435	61.833	1.00	64.40	8
ATOM	4425	OW6	WAT	X	53	36.689	9.501	46.403	1.00	43.78	8
ATOM	4426	OW7	WAT	X	53	13.785	14.234	21.394	1.00	46.49	8
ATOM	4427	OW8	WAT	X	53	44.108	8.308	6.121	1.00	74.38	8
ATOM	4428	OW9	WAT	X	53	37.095	13.297	47.553	1.00	92.89	8
ATOM	4429	OW0	WAT	X	54	60.222	38.361	56.675	1.00	71.18	8
ATOM	4430	OW1	WAT	X	54	43.676	52.104	52.067	1.00	52.01	8
ATOM	4431	OW2	WAT	X	54	13.472	23.519	26.526	1.00	85.06	8
ATOM	4432	OW3	WAT	X	54	26.573	48.774	55.241	1.00	63.24	8
ATOM	4433	OW4	WAT	X	54	38.373	54.655	25.877	1.00	61.51	8
ATOM	4434	OW5	WAT	X	54	40.109	29.004	7.323	1.00	50.80	8
ATOM	4435	OW6	WAT	X	54	40.897	28.228	33.474	1.00	55.10	8
ATOM	4436	OW8	WAT	X	54	26.359	57.407	32.671	1.00	74.31	8
ATOM	4437	OW9	WAT	X	54	15.383	36.694	13.336	1.00	63.49	8
ATOM	4438	OW0	WAT	X	55	25.637	23.526	51.791	1.00	62.36	8
ATOM	4439	OW1	WAT	X	55	47.868	37.197	21.724	1.00	98.01	8
ATOM	4440	OW2	WAT	X	55	48.664	28.592	20.875	1.00	61.42	8
ATOM	4441	OW3	WAT	X	55	22.182	11.543	42.550	1.00	50.93	8
ATOM	4442	OW4	WAT	X	55	14.290	33.767	23.519	1.00	43.45	8
ATOM	4443	OW5	WAT	X	55	49.254	21.261	57.388	1.00	74.77	8
ATOM	4444	OW6	WAT	X	55	32.072	50.437	56.442	1.00	84.60	8
ATOM	4445	OW7	WAT	X	55	6.861	26.478	7.012	1.00	69.24	8
ATOM	4446	OW8	WAT	X	55	36.069	6.771	2.277	1.00	89.64	8
ATOM	4447	OW9	WAT	X	55	60.239	29.387	37.677	1.00	64.46	8
ATOM	4448	OW1	WAT	X	56	46.693	15.300	46.504	1.00	37.40	8
ATOM	4449	OW2	WAT	X	56	47.685	47.802	26.981	1.00	44.40	8
ATOM	4450	OW3	WAT	X	56	21.472	47.007	15.910	1.00	70.01	8
ATOM	4451	OW4	WAT	X	56	2.967	21.682	5.603	1.00	60.74	8
ATOM	4452	OW5	WAT	X	56	62.723	25.567	58.195	1.00	45.51	8

SUBSTITUTE SHEET (RULE 26)

Appendix 1

ATOM	4453	OW6	WAT	X	56	53.874	20.460	35.843	1.00	60.27	8
ATOM	4454	OW7	WAT	X	56	34.043	6.968	31.691	1.00	54.01	8
ATOM	4455	OW8	WAT	X	56	20.830	41.835	12.224	1.00	100.00	8
ATOM	4456	OW9	WAT	X	56	16.599	30.946	13.916	1.00	37.38	8
ATOM	4457	OW0	WAT	X	57	44.358	21.696	24.084	1.00	64.44	8
ATOM	4458	OW1	WAT	X	57	9.788	43.318	30.716	1.00	90.76	8
ATOM	4459	OW2	WAT	X	57	65.207	28.476	57.189	1.00	72.19	8
ATOM	4460	OW3	WAT	X	57	20.871	4.547	-1.268	1.00	64.52	8
ATOM	4461	OW5	WAT	X	57	24.856	36.282	6.866	1.00	55.25	8
ATOM	4462	OW7	WAT	X	57	65.931	24.875	58.247	1.00	42.06	8
ATOM	4463	OW8	WAT	X	57	41.604	10.565	45.137	1.00	80.93	8
ATOM	4464	OW9	WAT	X	57	30.736	44.603	54.453	1.00	58.39	8
ATOM	4465	OW0	WAT	X	58	22.167	48.706	40.870	1.00	52.19	8
ATOM	4466	OW1	WAT	X	58	66.082	25.557	51.546	1.00	48.90	8
ATOM	4467	OW2	WAT	X	58	25.692	34.825	52.948	1.00	50.59	8
ATOM	4468	OW3	WAT	X	58	26.160	51.696	48.736	1.00	44.75	8
ATOM	4469	OW4	WAT	X	58	56.334	43.153	40.380	1.00	53.34	8
ATOM	4470	OW5	WAT	X	58	30.990	17.627	55.917	1.00	84.28	8
ATOM	4471	OW6	WAT	X	58	45.287	39.941	7.939	1.00	57.03	8
ATOM	4472	OW7	WAT	X	58	3.405	18.650	9.230	1.00	73.95	8
ATOM	4473	OW8	WAT	X	58	54.294	19.752	55.578	1.00	50.99	8
ATOM	4474	OW9	WAT	X	58	44.732	52.287	54.381	1.00	75.96	8
ATOM	4475	OW0	WAT	X	59	47.776	51.035	36.798	1.00	53.81	8
ATOM	4476	OW1	WAT	X	59	29.391	47.450	56.869	1.00	86.62	8
ATOM	4477	OW2	WAT	X	59	38.808	50.946	52.782	1.00	47.24	8
ATOM	4478	OW3	WAT	X	59	20.090	10.595	-7.477	1.00	69.34	8
ATOM	4479	OW4	WAT	X	59	30.700	10.315	45.674	1.00	63.75	8
ATOM	4480	OW5	WAT	X	59	60.018	46.795	44.900	1.00	57.35	8
ATOM	4481	OW6	WAT	X	59	46.214	52.834	49.312	1.00	67.99	8
ATOM	4482	OW7	WAT	X	59	56.880	28.891	60.457	1.00	85.53	8
ATOM	4483	OW8	WAT	X	59	36.201	48.379	58.178	1.00	71.18	8
ATOM	4484	OW9	WAT	X	59	35.313	2.318	16.129	1.00	66.51	8
ATOM	4485	OW0	WAT	X	60	34.944	58.828	34.422	1.00	69.27	8
ATOM	4486	OW1	WAT	X	60	47.891	40.270	60.882	1.00	62.61	8
ATOM	4487	OW2	WAT	X	60	20.100	54.046	30.414	1.00	91.37	8
ATOM	4488	OW3	WAT	X	60	0.668	22.084	15.126	1.00	45.99	8
ATOM	4489	OW4	WAT	X	60	50.911	50.933	54.227	1.00	71.78	8
ATOM	4490	OW5	WAT	X	60	50.514	44.428	38.574	1.00	67.41	8
ATOM	4491	OW6	WAT	X	60	31.208	54.171	26.648	1.00	65.99	8
ATOM	4492	OW7	WAT	X	60	49.541	38.319	60.498	1.00	49.78	8
ATOM	4493	OW8	WAT	X	60	23.270	55.339	31.653	1.00	66.17	8
ATOM	4494	OW9	WAT	X	60	46.551	15.109	50.163	1.00	87.28	8
ATOM	4495	OW0	WAT	X	61	65.999	24.860	47.686	1.00	57.42	8
ATOM	4496	OW1	WAT	X	61	30.573	36.197	57.967	1.00	51.73	8
ATOM	4497	OW2	WAT	X	61	3.779	13.380	-2.503	1.00	65.73	8
ATOM	4498	OW3	WAT	X	61	48.944	12.221	41.061	1.00	39.29	8
ATOM	4499	OW5	WAT	X	61	64.745	25.656	43.289	1.00	52.05	8
ATOM	4500	OW6	WAT	X	61	51.657	40.026	13.448	1.00	68.71	8
ATOM	4501	OW7	WAT	X	61	27.718	47.942	52.615	1.00	54.81	8
ATOM	4502	OW8	WAT	X	61	24.460	41.243	12.842	1.00	65.85	8
ATOM	4503	OW9	WAT	X	61	2.848	14.406	12.411	1.00	61.94	8
ATOM	4504	OW0	WAT	X	62	23.747	48.989	47.991	1.00	55.02	8
ATOM	4505	OW1	WAT	X	62	63.167	23.291	45.841	1.00	64.42	8
ATOM	4506	OW2	WAT	X	62	55.731	29.439	38.673	1.00	64.37	8
ATOM	4507	OW3	WAT	X	62	39.039	4.879	14.767	1.00	52.29	8
ATOM	4508	NA	ION	S	505	43.782	27.030	47.614	1.00	5.00	8
ATOM	4509	OW8	WAT	X	62	27.765	34.219	1.860	1.00	67.67	8
ATOM	4510	OW9	WAT	X	62	65.774	20.800	46.451	1.00	72.56	8
ATOM	4511	OW0	WAT	X	63	65.823	27.727	48.583	1.00	52.36	8
ATOM	4512	OW2	WAT	X	63	47.510	11.024	43.713	1.00	70.64	8
ATOM	4513	OW4	WAT	X	63	66.150	30.203	50.411	1.00	51.22	8
ATOM	4514	OW5	WAT	X	63	48.889	20.346	31.711	1.00	85.43	8
ATOM	4515	OW6	WAT	X	63	16.744	26.725	47.695	1.00	75.57	8
ATOM	4516	OW7	WAT	X	63	19.203	31.730	8.203	1.00	81.36	8
ATOM	4517	OW8	WAT	X	63	18.178	51.891	26.673	1.00	67.60	8
ATOM	4518	OW9	WAT	X	63	31.035	55.837	30.147	1.00	68.28	8
ATOM	4519	OW0	WAT	X	64	34.256	54.728	25.341	1.00	80.95	8
ATOM	4520	OW2	WAT	X	64	44.621	47.771	25.528	1.00	59.54	8
ATOM	4521	OW3	WAT	X	64	16.999	27.936	51.121	1.00	61.68	8
ATOM	4522	OW6	WAT	X	64	36.358	38.943	11.274	1.00	52.06	8
ATOM	4523	OW7	WAT	X	64	16.484	22.381	39.229	1.00	69.59	8
ATOM	4524	OW8	WAT	X	64	23.799	46.745	46.122	1.00	36.64	8
ATOM	4525	OW9	WAT	X	64	30.457	7.355	-1.129	1.00	72.94	8
ATOM	4526	OW0	WAT	X	65	19.222	33.502	3.190	1.00	50.09	8
ATOM	4527	OW1	WAT	X	65	46.509	18.371	25.238	1.00	62.10	8
ATOM	4528	OW5	WAT	X	65	32.283	10.295	-4.119	1.00	66.36	8
ATOM	4529	OW6	WAT	X	65	11.959	41.211	33.089	1.00	76.54	8
ATOM	4530	OW7	WAT	X	65	19.983	24.472	46.573	1.00	65.57	8
ATOM	4531	OW8	WAT	X	65	9.603	26.690	3.912	1.00	75.52	8
ATOM	4532	OW0	WAT	X	66	45.825	9.757	40.836	1.00	72.28	8
ATOM	4533	OW3	WAT	X	66	49.404	34.287	20.920	1.00	61.42	8
ATOM	4534	OW4	WAT	X	66	21.346	51.355	35.980	1.00	76.73	8
ATOM	4535	OW5	WAT	X	66	34.793	9.610	-4.714	1.00	67.39	8
ATOM	4536	OW6	WAT	X	66	6.006	27.070	13.534	1.00	83.61	8
ATOM	4537	OW0	WAT	X	67	57.091	33.822	60.700	1.00	78.52	8
ATOM	4538	OW1	WAT	X	67	3.688	25.711	4.813	1.00	69.62	8
ATOM	4539	OW3	WAT	X	67	11.853	27.880	7.921	1.00	58.69	8
ATOM	4540	OW5	WAT	X	67	35.486	56.715	40.693	1.00	63.30	8
ATOM	4541	OW8	WAT	X	67	20.467	20.497	41.249	1.00	43.89	8
ATOM	4542	OW9	WAT	X	67	37.508	57.667	34.228	1.00	57.61	8
ATOM	4543	OW0	WAT	X	68	8.621	27.294	14.147	1.00	69.67	8
ATOM	4544	OW1	WAT	X	68	3.733	19.033	3.659	1.00	55.12	8
ATOM	4545	OW2	WAT	X	68	18.954	18.854	32.541	1.00	55.87	8
ATOM	4546	OW3	WAT	X	68	25.346	2.504	4.877	1.00	67.33	8
ATOM	4547	OW4	WAT	X	68	34.927	1.355	1.837	1.00	66.26	8
ATOM	4548	OW5	WAT	X	68	47.719	47.565	30.106	1.00	61.60	8
ATOM	4549	OW6	WAT	X	68	58.933	17.613	53.979	1.00	67.71	8
ATOM	4550	OW0	WAT	X	69	16.418	40.606	47.124	1.00	65.35	8
ATOM	4551	OW2	WAT	X	69	33.051	35.235	6.368	1.00	61.68	8
ATOM	4552	OW3	WAT	X	69	10.404	2.233	-1.826	1.00	63.11	8
ATOM	4553	OW4	WAT	X	69	27.844	10.427	43.773	1.00	71.56	8
ATOM	4554	OW5	WAT	X	69	9.821	19.794	23.580	1.00	65.38	8
ATOM	4555	OW8	WAT	X	69	34.906	24.545	27.529	1.00	74.16	8
ATOM	4556	OW9	WAT	X	69	42.873	50.245	43.593	1.00	77.66	8
ATOM	4557	OW0	WAT	X	70	11.780	40.835	20.822	1.00	82.51	8
ATOM	4558	OW1	WAT	X	70	23.833	50.272	22.080	1.00	57.23	8

ATOM	4559	OW3	WAT	X	70	12.149	0.500	-0.175	1.00	100.00	8
ATOM	4560	OW4	WAT	X	70	24.781	48.147	16.489	1.00	53.74	8
ATOM	4561	OW5	WAT	X	70	45.295	18.629	15.166	1.00	66.52	8
ATOM	4562	OW8	WAT	X	70	16.273	24.172	43.929	1.00	86.28	8
ATOM	4563	OW2	WAT	X	71	14.692	0.299	4.588	1.00	76.24	8
ATOM	4564	OW3	WAT	X	71	56.655	45.988	46.443	1.00	74.53	8
ATOM	4565	OW4	WAT	X	71	44.653	15.572	21.500	1.00	81.92	8
ATOM	4566	OW6	WAT	X	71	13.915	34.012	32.549	1.00	76.95	8
ATOM	4567	OW1	WAT	X	72	18.894	23.324	28.037	1.00	69.01	8
ATOM	4568	OW2	WAT	X	72	25.942	27.526	52.380	1.00	80.30	8
ATOM	4569	OW3	WAT	X	72	20.444	43.760	44.743	1.00	57.92	8
ATOM	4570	OW5	WAT	X	72	56.463	15.927	56.362	1.00	90.66	8
ATOM	4571	OW6	WAT	X	72	67.258	38.530	40.380	1.00	67.91	8
ATOM	4572	OW2	WAT	X	73	13.119	23.916	-2.569	1.00	57.58	8
ATOM	4573	OW3	WAT	X	73	27.753	4.319	2.523	1.00	68.14	8
ATOM	4574	OW4	WAT	X	73	15.049	27.612	26.046	1.00	71.85	8
ATOM	4575	OW7	WAT	X	73	41.506	30.331	28.071	1.00	39.96	8
ATOM	4576	OW9	WAT	X	73	49.356	13.175	50.180	1.00	77.21	8
ATOM	4577	OW0	WAT	X	74	44.776	9.064	36.247	1.00	56.22	8
ATOM	4578	OW2	WAT	X	74	14.995	33.147	12.393	1.00	74.77	8
ATOM	4579	OW3	WAT	X	74	21.394	18.527	43.796	1.00	77.10	8
ATOM	4580	OW4	WAT	X	74	-0.275	3.244	2.071	1.00	89.93	8
ATOM	4581	OW5	WAT	X	74	32.705	3.566	1.290	1.00	100.00	8
ATOM	4582	OW6	WAT	X	74	23.871	44.907	16.023	1.00	71.10	8
ATOM	4583	OW8	WAT	X	74	41.289	9.005	3.932	1.00	71.97	8
ATOM	4584	OW2	WAT	X	75	38.329	57.673	44.241	1.00	64.90	8
ATOM	4585	OW5	WAT	X	75	18.910	30.958	52.593	1.00	93.30	8
ATOM	4586	OW6	WAT	X	75	68.020	36.610	50.288	1.00	86.49	8
ATOM	4587	OW2	WAT	X	76	22.139	39.199	7.275	1.00	71.53	8
ATOM	4588	OW3	WAT	X	76	58.720	42.672	38.660	1.00	68.73	8
ATOM	4589	OW5	WAT	X	76	61.482	44.540	47.192	1.00	77.48	8
ATOM	4590	OW9	WAT	X	76	22.107	41.072	47.776	1.00	60.73	8
ATOM	4591	OW2	WAT	X	77	2.634	-1.318	3.949	1.00	69.96	8
ATOM	4592	OW3	WAT	X	77	32.187	5.643	25.223	1.00	76.13	8
ATOM	4593	OW4	WAT	X	77	67.602	33.066	51.363	1.00	72.25	8
ATOM	4594	OW5	WAT	X	77	52.748	50.627	48.547	1.00	74.39	8
ATOM	4595	OW6	WAT	X	77	10.204	44.509	25.769	1.00	64.94	8
ATOM	4596	OW7	WAT	X	77	22.754	10.234	24.846	1.00	66.60	8
ATOM	4597	OW2	WAT	X	78	65.372	34.387	54.026	1.00	68.26	8
ATOM	4598	OW3	WAT	X	78	61.952	23.010	40.260	1.00	64.44	8
ATOM	4599	OW4	WAT	X	78	6.141	-0.725	6.920	1.00	63.43	8
ATOM	4600	OW6	WAT	X	78	62.946	40.127	37.159	1.00	74.61	8
ATOM	4601	OW2	WAT	X	79	57.524	45.787	43.333	1.00	68.47	8
ATOM	4602	OW3	WAT	X	79	27.601	6.844	22.540	1.00	100.00	8
ATOM	4603	OW4	WAT	X	79	13.772	31.115	20.743	1.00	57.33	8
ATOM	4604	OW5	WAT	X	79	58.663	23.880	36.310	1.00	71.62	8
ATOM	4605	OW6	WAT	X	79	49.511	45.784	34.237	1.00	64.41	8
ATOM	4606	OW2	WAT	X	80	42.349	10.479	16.376	1.00	86.89	8
ATOM	4607	OW3	WAT	X	80	64.430	36.390	57.479	1.00	81.60	8
ATOM	4608	OW4	WAT	X	80	51.348	32.222	6.850	1.00	86.83	8
ATOM	4609	OW6	WAT	X	80	28.165	8.846	38.088	1.00	71.08	8
ATOM	4610	OW8	WAT	X	80	65.757	27.493	53.760	1.00	48.10	8
ATOM	4611	OW1	WAT	X	81	45.249	12.674	37.874	1.00	50.64	8
ATOM	4612	OW2	WAT	X	81	13.341	34.872	38.349	1.00	64.64	8
ATOM	4613	OW3	WAT	X	81	51.626	42.754	59.455	1.00	87.45	8
ATOM	4614	OW5	WAT	X	81	17.748	40.786	43.576	1.00	81.62	8
ATOM	4615	OW6	WAT	X	81	40.981	31.297	32.687	1.00	92.90	8
ATOM	4616	OW7	WAT	X	81	36.339	42.304	57.906	1.00	54.44	8
ATOM	4617	OW0	WAT	X	82	52.150	44.557	55.907	1.00	81.29	8
ATOM	4618	OW1	WAT	X	82	44.696	27.699	29.800	1.00	66.84	8
ATOM	4619	OW2	WAT	X	82	15.369	42.073	36.641	1.00	87.69	8
ATOM	4620	OW4	WAT	X	82	44.262	38.613	61.725	1.00	74.79	8
ATOM	4621	OW5	WAT	X	82	10.887	37.555	22.160	1.00	77.71	8
ATOM	4622	OW6	WAT	X	82	57.317	26.895	38.482	1.00	54.04	8
ATOM	4623	OW1	WAT	X	83	1.485	10.546	14.639	1.00	49.60	8
ATOM	4624	OW2	WAT	X	83	44.383	11.585	44.954	1.00	69.75	8
ATOM	4625	OW4	WAT	X	83	13.091	19.080	23.540	1.00	84.10	8
ATOM	4626	OW5	WAT	X	83	49.664	18.609	50.424	1.00	79.36	8
ATOM	4627	OW6	WAT	X	83	-0.411	-0.186	6.219	1.00	73.91	8
ATOM	4628	OW1	WAT	X	84	-0.060	12.467	10.762	1.00	74.36	8
ATOM	4629	OW3	WAT	X	84	45.916	18.172	53.625	1.00	82.88	8
ATOM	4630	OW4	WAT	X	84	42.886	23.516	61.123	1.00	71.70	8
ATOM	4631	OW5	WAT	X	84	26.711	5.741	19.232	1.00	65.61	8
ATOM	4632	OW6	WAT	X	84	18.341	21.188	47.071	1.00	79.82	8
ATOM	4633	OW8	WAT	X	84	30.324	37.244	55.283	1.00	63.21	8
ATOM	4634	OW9	WAT	X	84	45.383	21.545	29.439	1.00	65.08	8
ATOM	4635	OW1	WAT	X	85	47.617	21.423	28.329	1.00	72.90	8
ATOM	4636	OW2	WAT	X	85	14.724	8.133	-4.054	1.00	80.41	8
ATOM	4637	OW4	WAT	X	85	14.404	38.900	34.440	1.00	73.60	8
ATOM	4638	OW5	WAT	X	85	30.311	39.411	56.032	1.00	72.07	8
ATOM	4639	OW1	WAT	X	86	38.750	51.931	56.443	1.00	83.88	8
ATOM	4640	OW2	WAT	X	86	28.737	50.755	56.620	1.00	78.91	8
ATOM	4641	OW3	WAT	X	86	38.447	9.203	1.111	1.00	60.02	8
ATOM	4642	OW4	WAT	X	86	63.955	18.750	55.290	1.00	75.30	8
ATOM	4643	OW5	WAT	X	86	28.437	41.435	56.329	1.00	77.99	8
ATOM	4644	OW6	WAT	X	86	27.951	49.707	19.814	1.00	80.66	8
ATOM	4645	OW7	WAT	X	86	33.978	8.299	40.249	1.00	69.22	8
ATOM	4646	OW9	WAT	X	86	17.498	1.498	10.616	1.00	71.37	8
ATOM	4647	OW1	WAT	X	87	1.278	15.798	6.438	1.00	70.87	8
ATOM	4648	OW3	WAT	X	87	37.174	55.549	52.513	1.00	69.91	8
ATOM	4649	OW4	WAT	X	87	68.146	21.047	55.397	1.00	70.79	8
ATOM	4650	OW5	WAT	X	87	24.655	52.548	24.459	1.00	72.31	8
ATOM	4651	OW6	WAT	X	87	46.009	24.086	33.287	1.00	79.02	8
ATOM	4652	OW9	WAT	X	87	50.195	14.529	36.835	1.00	65.15	8
ATOM	4653	OW2	WAT	X	88	29.201	3.240	-2.272	1.00	78.74	8
ATOM	4654	OW3	WAT	X	88	13.357	32.036	24.857	1.00	62.05	8
ATOM	4655	OW4	WAT	X	88	65.406	20.886	50.995	1.00	76.49	8
ATOM	4656	OW5	WAT	X	88	20.515	8.228	19.759	1.00	73.98	8
ATOM	4657	OW6	WAT	X	88	46.758	18.587	30.455	1.00	74.75	8
ATOM	4658	OW2	WAT	X	89	49.679	43.124	20.824	1.00	80.84	8
ATOM	4659	OW3	WAT	X	89	60.303	44.435	40.737	1.00	70.62	8
ATOM	4660	OW4	WAT	X	89	13.240	-1.159	9.184	1.00	78.53	8
ATOM	4661	OW5	WAT	X	89	61.700	19.538	53.061	1.00	64.93	8
ATOM	4662	OW6	WAT	X	89	24.291	28.301	0.472	1.00	69.68	8
ATOM	4663	OW0	WAT	X	90	27.964	24.098	-2.600	1.00	64.61	8
ATOM	4664	OW1	WAT	X	90	22.140	24.413	52.912	1.00	67.47	8

ATOM	4665	OW3	WAT	X	90	39.112	6.740	5.054	1.00	66.72	8
ATOM	4666	OW4	WAT	X	90	43.364	57.890	49.964	1.00	71.30	8
ATOM	4667	OW6	WAT	X	90	16.187	17.842	27.844	1.00	71.63	8
ATOM	4668	OW7	WAT	X	90	22.913	3.223	6.101	1.00	63.34	8
ATOM	4669	OW0	WAT	X	91	0.373	23.417	18.644	1.00	68.95	8
ATOM	4670	OW1	WAT	X	91	19.144	22.297	52.147	1.00	68.45	8
ATOM	4671	OW2	WAT	X	91	46.750	22.374	17.228	1.00	68.56	8
ATOM	4672	OW3	WAT	X	91	50.310	39.246	9.155	1.00	68.48	8
ATOM	4673	OW5	WAT	X	91	14.832	31.811	-1.674	1.00	65.32	8
ATOM	4674	OW6	WAT	X	91	39.568	22.971	59.682	1.00	94.75	8
ATOM	4675	OW0	WAT	X	92	28.305	37.474	53.688	1.00	64.82	8
ATOM	4676	OW1	WAT	X	92	60.842	35.037	35.557	1.00	68.20	8
ATOM	4677	OW3	WAT	X	92	38.306	2.043	9.940	1.00	74.71	8
ATOM	4678	OW4	WAT	X	92	37.932	10.010	23.873	1.00	62.54	8
ATOM	4679	OW5	WAT	X	92	37.872	59.284	31.560	1.00	64.40	8
ATOM	4680	OW8	WAT	X	92	16.587	37.900	45.458	1.00	57.48	8
ATOM	4681	OW2	WAT	X	93	24.426	6.991	31.450	1.00	62.04	8
ATOM	4682	OW3	WAT	X	93	15.322	46.823	24.885	1.00	68.48	8
ATOM	4683	OW5	WAT	X	93	18.754	23.194	42.946	1.00	69.72	8
ATOM	4684	OW6	WAT	X	93	20.937	46.805	43.439	1.00	65.25	8
ATOM	4685	OW8	WAT	X	93	28.767	42.761	53.085	1.00	51.35	8
ATOM	4686	OW0	WAT	X	94	32.517	16.473	33.381	1.00	60.16	8
ATOM	4687	OW2	WAT	X	94	26.635	4.800	29.351	1.00	63.33	8
ATOM	4688	OW3	WAT	X	94	1.194	4.216	9.172	1.00	60.36	8
ATOM	4689	OW4	WAT	X	94	25.652	19.885	-5.299	1.00	58.09	8
ATOM	4690	OW5	WAT	X	94	43.661	12.692	20.184	1.00	65.23	8
ATOM	4691	OW6	WAT	X	94	17.439	46.586	41.518	1.00	66.21	8
ATOM	4692	OW7	WAT	X	94	35.133	15.487	30.639	1.00	49.75	8
ATOM	4693	OW8	WAT	X	94	36.346	8.698	18.844	1.00	48.58	8
ATOM	4694	OW0	WAT	X	95	30.818	8.165	40.656	1.00	56.86	8
ATOM	4695	OW1	WAT	X	95	40.089	21.776	55.765	1.00	53.69	8
ATOM	4696	OW2	WAT	X	95	18.639	14.065	-5.612	1.00	55.94	8
ATOM	4697	OW3	WAT	X	95	51.587	38.457	41.331	1.00	56.04	8
ATOM	4698	OW4	WAT	X	95	50.107	29.401	17.255	1.00	56.00	8
ATOM	4699	OW5	WAT	X	95	8.218	14.744	20.596	1.00	56.95	8
ATOM	4700	OW6	WAT	X	95	40.674	47.760	57.927	1.00	54.91	8

CLAIMS

1. A method of constructing a variant of a parent Termamyl-like α-amylase, which variant has α-amylase activity and at least one altered property as compared to said parent α-amylase, which method comprises

i) analysing the structure of the parent Termamyl-like α-amylase to identify at least one amino acid residue or at least one structural part of the Termamyl-like α-amylase structure, which amino acid residue or structural part is believed to be of relevance for altering said property of the parent Termamyl-like α-amylase (as evaluated on the basis of structural or functional considerations),

ii) constructing a Termamyl-like α-amylase variant, which as compared to the parent Termamyl-like α-amylase, has been modified in the amino acid residue or structural part identified in i) so as to alter said property, and

iii) testing the resulting Termamyl-like α-amylase variant for said property.

2. The method according to claim 1, wherein the property to be altered is selected from the group consisting of substrate specificity, substrate binding, substrate cleavage pattern, temperature stability, pH dependent activity, pH dependent stability (especially increased stability at low (e.g. pH<6) or high (e.g. pH>9) pH values), stability towards oxidation, Ca^{2+}-dependency and specific activity.

3. The method according to claim 1 or 2, wherein the property to be altered is the calcium ion dependency and the structural part to be modified is selected from the group consisting of the C domain, the interface between the A and B domain, the interface between the A and C domain, or the interaction to a calcium binding site of the Termamyl-like α-amylase.

4. The method according to claim 1 or 2, wherein the property to be altered is the substrate cleavage pattern and the structural part to be modified is located within 10Å from an amino acid residue of the substrate binding site.

5. A method of constructing a variant of a parent Termamyl-like α-amylase, which variant has α-amylase activity and one or more altered properties as compared to said parent α-amylase, which method comprises

i) comparing the three-dimensional structure of the Termamyl-like α-amylase with the structure of a non-Termamyl-like α-amylase,

ii) identifying a part of the Termamyl-like α-amylase structure which is different from the non-Termamyl-like α-amylase structure and which from structural or functional considerations is contemplated to be responsible for differences in one or more properties of the Termamyl-like and non-Termamyl-like α-amylase, and

iii) modifying the part of the Termamyl-like α-amylase identified in ii) whereby a Termamyl-like α-amylase variant is obtained, one or more properties of which differ from the parent Termamyl-like α-amylase.

6. The method according to claim 6, wherein, in step iii), the part of the Termamyl-like α-amylase is modified so as to ressemble the corresponding part of the non-Termamyl-like α-amylase.

7. The method according to claim 5 or 6, wherein, in step iii), the modification is accomplished by deleting one or more amino acid residues of the part of the Termamyl-like α-amylase to be modified; by replacing one or more amino acid residues of the part of the Termamyl-like α-amylase to be modified with the amino acid residues occupying corresponding positions in the non-Termamyl-like α-amylase; or by insertion of one or more amino acid residues present in the non-Termamyl-like α-amylase into a corresponding position in the Termamyl-like α-amylase.

8. The method according to any of claims 5-7, wherein the non-Termamyl-like α-amylase structure is the structure of a fungal α-amylase or a mammalian α-amylase.

9. The method according to claim 8, wherein the non-Termamyl-like α-amylase is the *Aspergillus oryzae* TAKA α-amylase, the *A. niger* acid α-amylase, the *Bacillus subtilis* α-amylase or the pig pancreatic α-amylase.

10. The method according to any of claims 1-9, wherein the parent Termamyl-like α-amylase is derived from a strain of *Bacillus*.

11. The method according to claim 10, wherein the parent α-amylase is derived from a strain of a *B. licheniformis*, *B. amyloliquefaciens*, *B. stearothermophilus* or a strain from an alkalophilic *Bacillus* sp. such as NCIB 12289, NCIB 12512 or NCIB 12513.

12. The method according to any of claims 1-11, wherein the parent α-amylase is a hybrid α-amylase comprising a combination of partial amino acid sequences derived from at least two α-amylases, of which one is a Termamyl-like α-amylase and the other(s) are, e.g., from a microbial and/or a mammalian α-amylase.

13. The method according to any of claims 5-12, wherein the part of the parent Termamyl-like α-amylase to be modified and identified in step ii) is loop 1, loop 2, loop 3 and/or loop 8 of the parent α-amylase.

13. A method of constructing a variant of a parent Termamyl-like α-amylase, which has a decreased calcium ion dependency as compared to said parent, which method comprises:

i) identifying an amino acid residue within 10Å from a Ca^{2+} binding site of a Termamyl-like α-amylase in a model of the three-dimensional structure of said α-amylase, which from

structural or functional considerations is believed to be responsible for a non-optimal calcium ion interaction,
ii) constructing a variant in which said amino acid residue is replaced with another amino acid residue which from structural or functional considerations is believed to be important for establishing a higher Ca^{2+} binding affinity, and
iii) testing the Ca^{2+} dependency of the resulting Termamyl-like α-amylase variant.

14. A method of constructing a variant of a parent Termamyl-like α-amylase which variant has α-amylase activity and an altered pH dependent activity, which method comprises

i) in a three-dimensional structure of the Termamyl-like α-amylase in question, identifying an amino acid residue within 15Å from an active site residue, in particular 10Å from an active site residue, which amino acid residue is contemplated to be involved in electrostatic or hydrophobic interactions with an active site residue,

ii) replacing, in the structure, said amino acid residue with an amino acid residue which changes the electrostatic and/or hydrophobic surroundings of an active site residue and evaluating the accomodation of the amino acid residue in the structure,

iii) optionally repeating step i) and/or ii) until an amino acid replacement has been identified which is accomodated into the structure,

iv) constructing a Termamyl-like α-amylase variant resulting from steps i), ii) and optionally iii) and testing the pH dependent activity of said variant.

15. A method of increasing the thermostability and/or altering the temperature optimum of a parent Termamyl-like α-amylase, which method comprises

i) identifying an internal hole or a crevice of the parent Termamyl-like α-amylase in the three-dimensional structure of said α-amylase,

ii) replacing, in the structure, one or more amino acid residues in the neighbourhood of the hole or crevice identified in i) with another amino acid residue which from structural or functional considerations is believed to increase the hydrophobic interaction and to fill out or reduce the size of the hole or crevice,

iii) constructing a Termamyl-like α-amylase variant resulting from step ii) and testing the thermostability and/or temperature optimum of the variant.

16. A method of constructing a variant of a Termamyl-like α-amylase which has a reduced ability to cleave a substrate close to the branching point, which method comprises

i) identifying the substrate binding area of the parent Termamyl-like α-amylase in a model of the three-dimensional structure of said α-amylase,

ii) replacing, in the model, one or more amino acid residues of the substrate binding area of the cleft identified in i), which is/are believed to be responsible for the cleavage pattern of the parent α-amylase, with another amino acid residue which from structural considerations is believed to result in an altered substrate cleavage pattern, or deleting one or more amino acid residues of the substrate binding area contemplated to introduce favourable interactions to the substrate or adding one or more amino acid residues to the substrate binding area contemplated to introduce favourable interactions to the substrate, and

iii) constructing a Termamyl-like α-amylase variant resulting from step ii) and testing the substrate cleavage pattern of the variant.

17. The method according to any of the preceeding claims, in which the α-amylase variant is obtained by cultivating a

microorganism comprising a DNA sequence encoding the variant under conditions which are conducive for producing the variant, and optionally subsequently recovering the variant from the resulting culture broth.

18. A variant of a parent Termamyl-like α-amylase, in which variant at least one amino acid residue of the parent α-amylase, which is/are present in a fragment corresponding to the amino acid fragment 44-57 of the amino acid sequence of SEQ ID No. 4, has been deleted or replaced with one or more amino acid residues which is/are present in a fragment corresponding to the amino acid fragment 66-84 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has been added using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α-amylase as a template.

19. A variant of a parent Termamyl-like α-amylase, which variant has a region which, when the amino acid sequence of variant is aligned most closely with the amino acid sequence of the said parent α-amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No 4, the said region having at least 80% sequence homology with the part of SEQ ID No 10 extending from residue Z to residue V of SEQ ID No 10, wherein

X is the amino acid residue occupying position 44, 45, 46, 47 or 48 of SEQ ID No. 4,

Y is the amino acid residue occupying position 51, 52, 53, 54, 55, 56 or 57 of SEQ ID No. 4,

Z is the amino acid residue occupying position 66, 67, 68, 69 or 70 of SEQ ID No. 10, and

V is the amino acid residue occupying position 78, 79, 80, 81, 82, 83 or 84 of SEQ ID No. 10.

20. The variant according to claim 18 or 19, wherein X is the amino acid residue occupying position 48 and Y the amino acid residue occupying position 51 of SEQ ID NO 4 and Z is the amino

acid residue occupying position 70 and V the amino acid residue occupying position 78 in SEQ ID No 10.

21. A variant of a parent Termamyl-like α-amylase, in which variant at least one of the amino acid residues of the parent α-amylase, which is/are present in an amino acid fragment corresponding to the amino acid fragment 195-202 of the amino acid sequence of SEQ ID No. 4, has been deleted or replaced with one or more of the amino acid residues which is/are present in an amino acid fragment corresponding to the amino acid fragment 165-177 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has been added using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α-amylase as a template.

22. A variant of a parent Termamyl-like α-amylase, which variant has a region which, when the amino acid sequence of variant is aligned most closely with the amino acid sequence of the said parent α-amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No 4, the said region having at least 80%, such as 90% sequence homology with the part of SEQ ID No 10 extending from residue Z to residue V of SEQ ID No 10, wherein

X is the amino acid occupying position 195 or 196 of SEQ ID No. 4,

Y is the amino acid residue occupying position 198, 199, 200, 201, or 202 of SEQ ID No. 4,

Z is the amino acid residue occupying position 165 or 166 of SEQ ID No. 10, and

V is the amino acid residue occupying position 173, 174, 175, 176 or 177 of SEQ ID No. 10.

23. The variant according to claim 21 or 22, in which the amino acid fragment of the parent α-amylase, which corresponds to

amino acid residues 196-198 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino acid residues 166-173 of the amino acid sequence shown in SEQ ID No. 10.

24. A variant of a parent Termamyl-like α-amylase, in which variant at least one of the amino acid residues of the parent α-amylase, which is/are present in a fragment corresponding to the amino acid fragment 117-185 of the amino acid sequence of SEQ ID No. 4, has/have been deleted or replaced with one or more of the amino acid residues, which is/are present in an amino acid fragment corresponding to the amino acid fragment 98-210 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has been added using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α-amylase as a template.

25. A variant of a parent Termamyl-like α-amylase, which variant has a region which, when the amino acid sequence of variant is aligned most closely with the amino acid sequence of the said parent α-amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No 4, the said region having at least 80%, such as at least 90% sequence homology with the part of SEQ ID No 10 extending from residue Z to residue V of SEQ ID No 10, wherein

X is the amino acid occupying position 117, 118, 119, 120 or 121 of SEQ ID No. 4,

Y is the amino acid occupying position 181, 182, 183, 184 or 185 of SEQ ID No. 4,

Z is the amino acid occupying position 98, 99, 100, 101, 102 of SEQ ID No. 10, and

V is the amino acid occupying position 206, 207, 208, 209 or 210 of SEQ ID No. 10.

26. The variant according to claim 24 or 25, in which an amino acid fragment of the parent α-amylase, which corresponds to amino acid residues 121-181 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino acid residues 102-206 of the amino acid sequence shown in SEQ ID No. 10.

27. A variant of a parent Termamyl-like α-amylase, in which variant at least one of the amino acid residues of the parent α-amylase, which is/are present in a fragment corresponding to the amino acid fragment 117-181 of the amino acid sequence of SEQ ID No. 4, has/have been deleted or replaced with one or more of the amino acid residues, which is/are present in an amino acid fragment corresponding to the amino acid fragment to 98-206 of the amino acid sequence shown in SEQ ID No. 10, or in which one or more additional amino acid residues has been added using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α-amylase as a template.

28. A variant of a parent Termamyl-like α-amylase, which variant has a region which, when the amino acid sequence of variant is aligned most closely with the amino acid sequence of the said parent α-amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No 4, the said region having at least 80%, such as at least 90% sequence homology with the part of SEQ ID No 10 extending from residue Z to residue V of SEQ ID No 10, wherein

X is the amino acid occupying position 117, 118, 119, 120 or 121 of SEQ ID No. 4,

Y is the amino acid occupying position 174, 175, 176 or 177 of SEQ ID No. 4,

Z is the amino acid occupying position 98, 99, 100, 101, 102 of SEQ ID No. 10, and

V is the amino acid occupying position 199, 200, 201 or 202 of SEQ ID No. 10.

29. The variant according to claim 27 or 28, in which the amino acid fragment of the parent α-amylase, which corresponds to amino acid residues 121-174 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino acid residues 102-199 of the amino acid sequence shown in SEQ ID No. 10.

30. A variant of a parent Termamyl-like α-amylase, in which variant at least one of the amino acid residues of the parent α-amylase, which is/are present in an amino acid fragment corresponding to the amino acid fragment 12-19 of the amino acid sequence of SEQ ID No. 4, has/have been deleted or replaced with one or more of the amino acid residues, which is/are present in an amino acid fragment which corresponds to the amino acid fragment 28-42 of SEQ ID No. 10, or in which one or more additional amino acid residues has/have been inserted using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α-amylase as a template.

31. A variant of a parent Termamyl-like α-amylase, which variant has a region which, when the amino acid sequence of variant is aligned most closely with the amino acid sequence of the said parent α-amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No 4, the said region having at least 80%, such as at least 90% sequence homology with the part of SEQ ID No 10 extending from residue Z to residue V of SEQ ID No 10, wherein

X is the amino acid occupying position 12, 13 or 14 of SEQ ID No. 4,

Y is the amino acid occupying position 15, 16, 17, 18 or 19 of SEQ ID No. 4,

Z is the amino acid occupying position 28, 29, 30, 31 or 32 of SEQ ID No. 10, and

V is an amino acid residue corresponding to the amino acid occupying position 38, 39, 40, 41 or 42 of SEQ ID No. 10.

32. The variant according to claim 30 or 31, in which the amino acid fragment of the parent α-amylase, which corresponds to amino acid residues 14-15 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino acid residues 32-38 of the amino acid sequence shown in SEQ ID No. 10.

33. A variant of a parent Termamyl-like α-amylase, in which variant at least one of the amino acid residues of the parent α-amylase, which is present in a fragment corresponding to amino acid residues 7-23 of the amino acid sequence of SEQ ID No. 4, has/have been deleted or replaced with one or more amino acid residues, which is/are present in an amino acid fragment corresponding to amino acid residues 13-45 of the amino acid sequence shown in SEQ ID No. 10, or or in which one or more additional amino acid residues has/have been inserted using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α-amylase as a template.

34. A variant of a parent Termamyl-like α-amylase, which variant has a region which, when the amino acid sequence of variant is aligned most closely with the amino acid sequence of the said parent α-amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No 4, the said region having at least 80%, such as at least 90% sequence homology with the part of SEQ ID No 10 extending from residue Z to residue V of SEQ ID No 10, wherein

X is the amino acid occupying position 7 or 8 of SEQ ID No. 4,

Y is the amino acid occupying position 18, 19, 20, 21, 22 or 23 of SEQ ID No. 4,

Z is the amino acid occupying position 13 or 14 of SEQ ID No. 10, and

V is the amino acid occupying position 40, 41, 42, 43, 44 or 45 of SEQ ID No. 10.

35. The variant according to claim 33 or 34, in which the amino acid fragment of the parent α-amylase, which corresponds to amino acid residues 8-18 of SEQ ID No. 4, has been replaced with the amino acid fragment corresponding to amino acid residues 14-40 of the amino acid sequence shown in SEQ ID No. 10.

36. A variant of a parent Termamyl-like α-amylase, in which variant at least one of the amino acid residues of the parent α-amylase, which is present in a fragment corresponding to amino acid residues 322-346 of the amino acid sequence of SEQ ID No. 2, has/have been deleted or replaced with one or more amino acid residues, which is/are present in an amino acid fragment corresponding to amino acid residues 291-313 of the amino acid sequence shown in SEQ ID No. 10, or or in which one or more additional amino acid residues has/have been inserted using the relevant part of SEQ ID No. 10 or a corresponding part of another Fungamyl-like α-amylase as a template.

37. A variant of a parent Termamyl-like α-amylase, which variant has a region which, when the amino acid sequence of variant is aligned most closely with the amino acid sequence of the said parent α-amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No 2, the said region having at least 80% sequence homology with the part of SEQ ID No 10 extending from residue Z to residue V of SEQ ID No 10, wherein

X is the amino acid occupying position 322, 323, 324 or 325 of SEQ ID No. 2,

Y is the amino acid occupying position 343, 344, 345 or 346 of SEQ ID No. 2,

Z is the amino acid occupying position 291, 292, 293 or 294 of SEQ ID No. 10, and

V is the amino acid occupying position 310, 311, 312 or 313 of SEQ ID No. 10.

38. The variant according to claim 36 or 37, in which the amino acid fragment of the parent α-amylase, which corresponds to amino acid residues 325-345 of SEQ D No. 2, has been replaced with the amino acid fragment corresponding to amino acid residues 294-313 of the amino acid sequence shown in SEQ ID No. 10.

39. A variant of a parent Fungamyl-like α-amylase, in which variant at least one of the amino acid residues of the parent α-amylase, which is/are present in an amino acid fragment corresponding to amino acid residues 291-313 of the amino acid sequence of SEQ ID No. 10, has/have been deleted or replaced with one or more of the amino acid residues, which is/are present in an amino acid fragment corresponding to amino acid residues 98-210 of the amino acid sequence shown in SEQ ID No. 4, or in which one or more additional amino acid residues has/have been inserted using the relevant part of SEQ ID No. 4 or a corresponding part of another Termamyl-like α-amylase as a template.

40. A variant of a parent Fungamyl-like α-amylase, which variant has a region which, when the amino acid sequence of variant is aligned most closely with the amino acid sequence of the said parent α-amylase, occupies the same position as the portion from residue X to residue Y of SEQ ID No 10, the said region having at least 80%, such as at least 90% sequence homology with the part of SEQ ID No 10 extending from residue Z to residue V of SEQ ID No 4, wherein

X is the amino acid occupying position 117, 118, 119, 120 or 121 of SEQ ID No. 10,

Y is the amino acid occupying position 181, 182, 183, 184 or 185 of SEQ ID No. 10,

Z is the amino acid occupying position 98, 99, 100, 101 or 102 of SEQ ID No. 4, and

V is the amino acid occupying position 206, 207, 208, 209 or 210 of SEQ ID No. 4.

41. The variant according to claim 39 or 40, in which the amino acid fragment of the parent α-amylase, which corresponds to amino acid residues 121-181 of SEQ ID No. 10, has been replaced with the amino acid fragment corresponding to amino acid residues 102-206 of the amino acid sequence shown in SEQ ID No. 4.

42. A variant according to any of claims 39-41, in which the the amino acid fragment of the parent α-amylase, which corresponds to amino acid residues 121-174 of SEQ ID No. 10, has been replaced with the amino acid fragment corresponding to amino acid residues 102-199 of the amino acid sequence shown in SEQ ID No. 4.

43. A variant of a parent Fungamyl-like α-amylase, in which an amino acid fragment corresponding to amino acid residues 181-184 of the amino acid sequence shown in SEQ ID No. 10 has been deleted.

45. A variant of a parent Termamyl-like α-amylase, which exhibits α-amylase activity and which has a decreased Ca^{2+} dependency as compared to the parent α-amylase.

46. A variant according to claim 45, which comprises a mutation in a position corresponding to at least one of the following positions in SEQ ID NO 2:
N104, A349, I479, L346, I430, N457, K385, F350, I411, H408 or G303, in particular a mutation corrsponding to
N104D;
A349C+I479C;
L346C+I430C;
N457D,E;
N457D,E+K385R;
F350D,E+I430R,K;
F350D,E+I411R,K;

H408Q,E,N,D; and/or
G303N,D,Q,E.

47. A variant of a parent Termamyl-like α-amylase which exhibits a higher activity below the pH optimum than the parent α-amylase, which variant comprises a mutation of an amino acid residue corresponding to at least one of the following positions of the *B. licheniformis* α-amylase (SEQ ID NO 2): E336, Q333, P331, I236, V102, A232, I103, L196, in particular at least one of the following mutations:
E336R,K;
Q333R,K; P331R,K;
V102R,K,A,T,S,G;
I236K,R,N;
I103K,R;
L196K,R; and/or
A232T,S,G.

48. A variant of a parent Termamyl-like α-amylase which exhibits a higher activity above the pH optimum than the parent α-amylase, which variant comprises a mutation of an amino acid residue corresponding to at least one of the following positions of the *B. licheniformis* α-amylase (SEQ ID NO 2): N236, H281 and/or Y273, in particular one of the follwoing mutations:
N326I,Y,F,L,V;
H281F,I,L; and/or
Y273F,W.

49. A variant of a parent Termamyl-like α-amylase which exhibits α-amylase activity and which has an increased thermostability and/or altered temperature optimum as compared to the parent α-amylase, which variant comprises a mutation of an amino acid residue corresponding to at least one of the following positions of the *B. licheniformis* α-amylase (SEQ ID NO 2):

L61, Y62, F67, K106, G145, I212, S151, R214, Y150, F143, R146, L241, I236, L7, V259, F284, F350, F343, L427 and/or V481, in particular at least one of the following mutations:
L61W,V,F;
Y62W;
F67W;
K106R,F,W;
G145F,W
I212F,L,W,Y,R,K;
S151 replaced with any other amino acid residue and in particular with F,W,I or L;
R214W;
Y150R,K;
F143W;
R146W;
L241I,F,Y,W;
I236L,F,W,Y;
L7F,I,W;
V259F,I,L;
F284W;
F350W;
F343W;
L427F,L,W; and/or
V481,F,I,L,W.

50. A variant of a parent Termamyl-like α-amylase, which exhibits α-amylase activity and which has a reduced capability of cleaving an oligo-saccharide substrate close to the branching point as compared to the parent α-amylase, which variant comprises a mutation of an amino acid residue corresponding to at least one of the following positions of the *B. licheniformis* α-amylase (SEQ ID NO 2):

V54, D53, Y56, Q333 and/or G57, in particular at least one of the following mutations:
V54L,I,F,Y,W,R,K,H,E,Q;
D53L,I,F,Y,W;
Y,56W;

Q333W; and/or
G57 to all possible amino acid residues.

51. The variant according to any of claims 17-50, wherein one or more proline residues present in the amino acid residues with which the parent α-amylase is modified are replaced with a non-proline residue such as alanine.

52. The variant according to any of claims 17-51, wherein one or more cysteine residues present in the amino acid residues with which the parent α-amylase is modified are replaced with a non-cysteine residue such as alanine.

53. A DNA construct comprising a DNA sequence encoding an α-amylase variant according to any of claims 17-52.

54. A recombinant expression vector which carries a DNA construct according to Claim 53.

55. A cell which is transformed with a DNA construct according to Claim 53 or a vector according to Claim 54.

56. A cell according to Claim 55, which is a microorganism.

57. A cell according to Claim 56, which is a bacterium or a fungus.

58. The cell according to Claim 57, which is a grampositive bacterium such as *Bacillus subtilis*, *Bacillus licheniformis*, *Bacillus lentus*, *Bacillus brevis*, *Bacillus stearothermophilus*, *Bacillus alkalophilus*, *Bacillus amyloliquefaciens*, *Bacillus coagulans*, *Bacillus circulans*, *Bacillus lautus* or *Bacillus thuringiensis*.

59. Use of an α-amylase variant according to any of claims 17-52 for washing and/or dishwashing.

60. Use of an α-amylase variant according to any of claims 17-52 for desizing.

61. Use of an α-amylase variant according to any of claims 17-52 for starch liquefaction.

62. A detergent additive comprising an α-amylase variant according to any of claims 17-52, optionally in the form of a non-dusting granulate, stabilised liquid or protected enzyme.

63. A detergent additive according to Claim 62 which contains 0.02-200 mg of enzyme protein/g of the additive.

64. A detergent additive according to Claim 62 or 63, which additionally comprises another enzyme such as a protease, a lipase, a peroxidase, another amylolytic enzyme and/or a cellulase.

65. A detergent composition comprising an α-amylase variant according to any of claims 17-52.

66. A detergent composition according to Claim 65 which additionally comprises another enzyme such as a protease, a lipase, a peroxidase, another amylolytic enzyme and/or a cellulase.

67. A manual or automatic dishwashing detergent composition comprising an α-amylase variant according to any of claims 17-52.

68. A dishwashing detergent composition according to Claim 67 which additionally comprises another enzyme such as a protease, a lipase, a peroxidase, another amylolytic enzyme and/or a cellulase.

69. A manual or automatic laundry washing composition comprising an α-amylase variant according to any of claims 17-52.

70. A laundry washing composition according to Claim 69, which additionally comprises another enzyme such as a protease, a lipase, a peroxidase, an amylolytic enzyme and/or a cellulase.

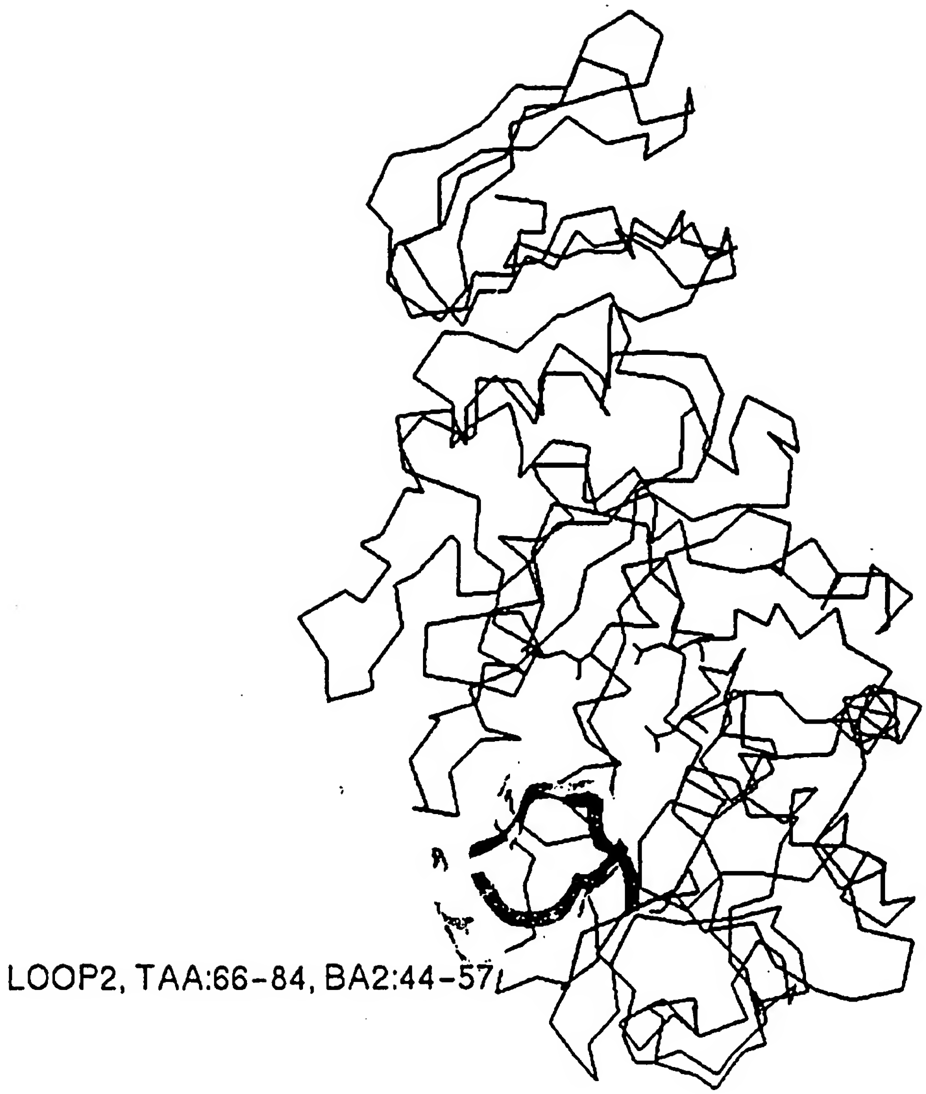

Fig. 1

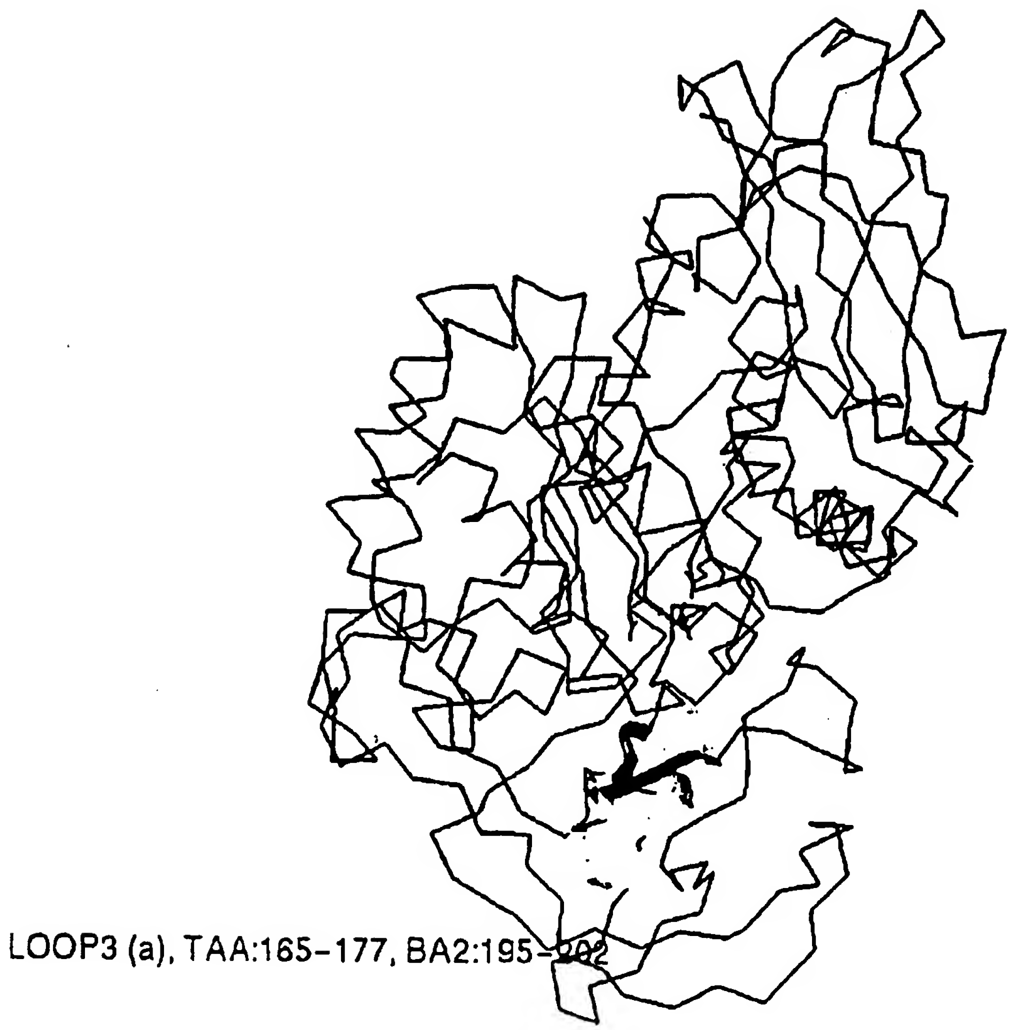

Fig. 2

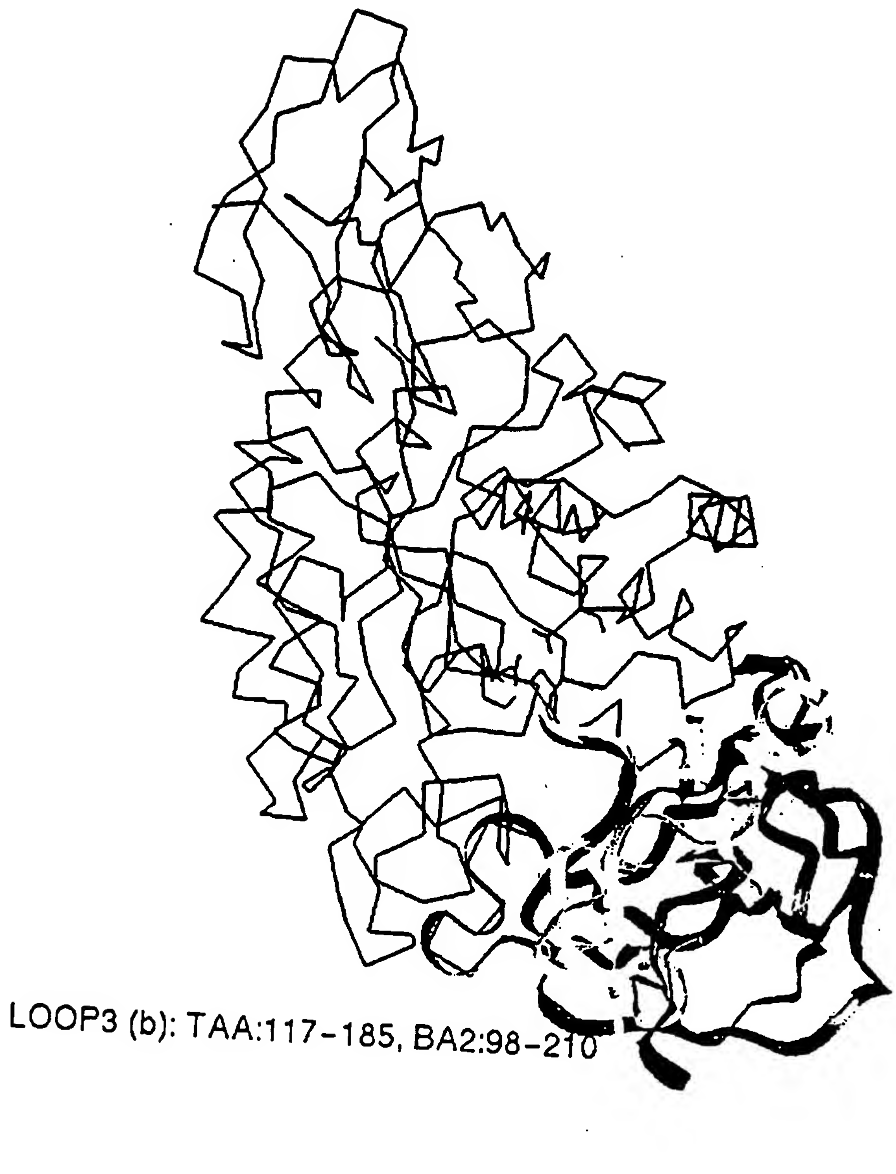

Fig. 3

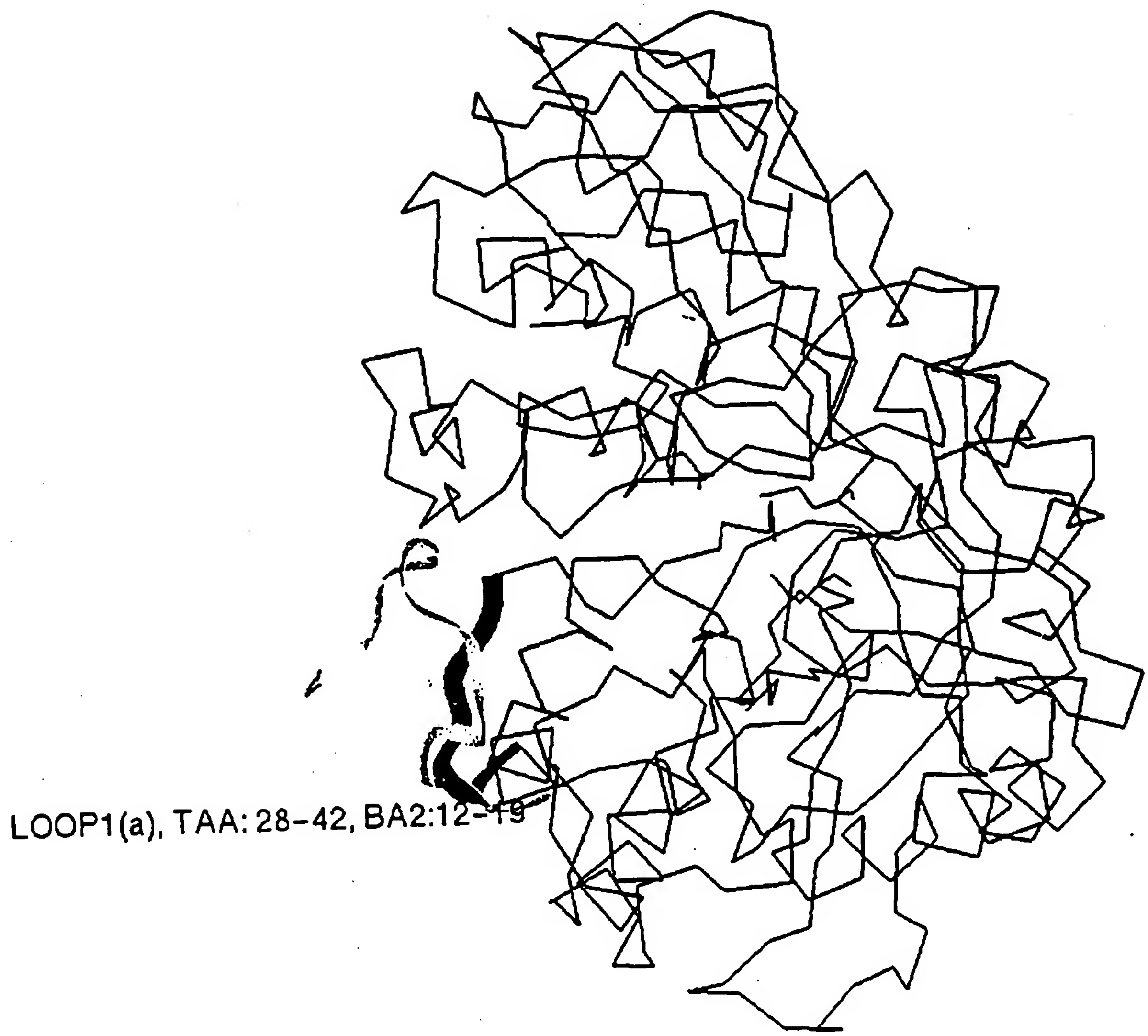

Fig. 4

Fig. 5

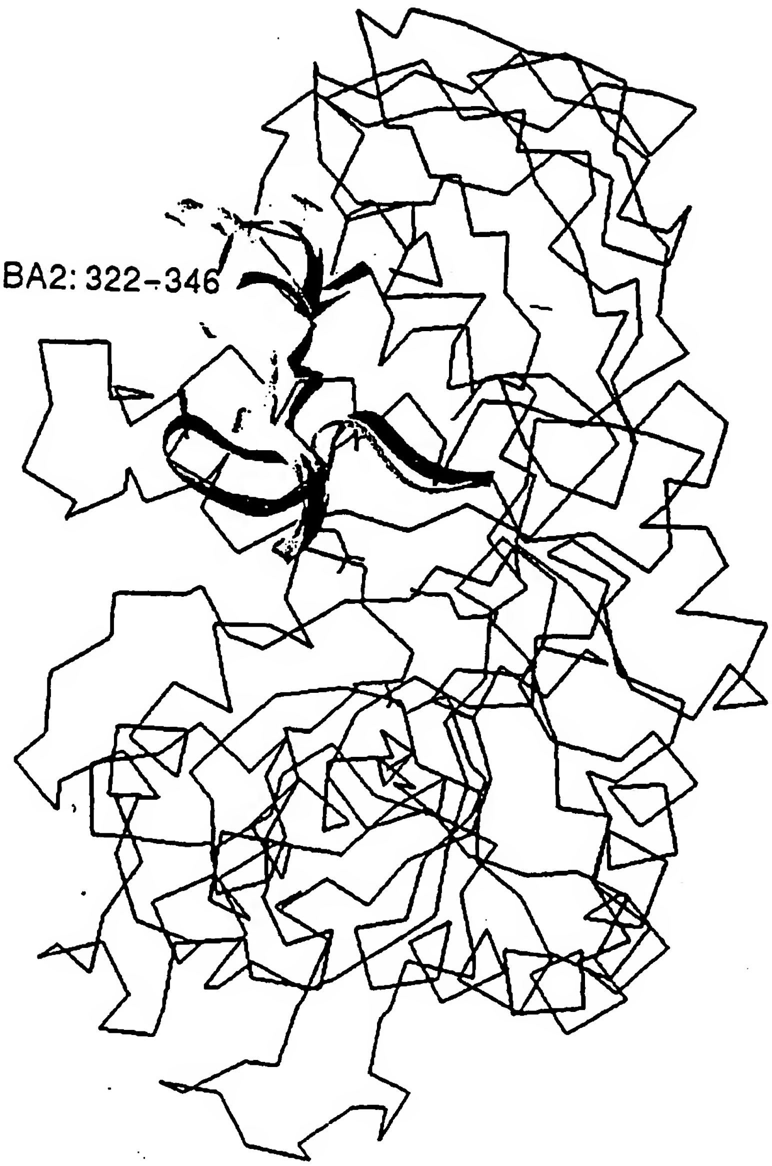

Fig. 6

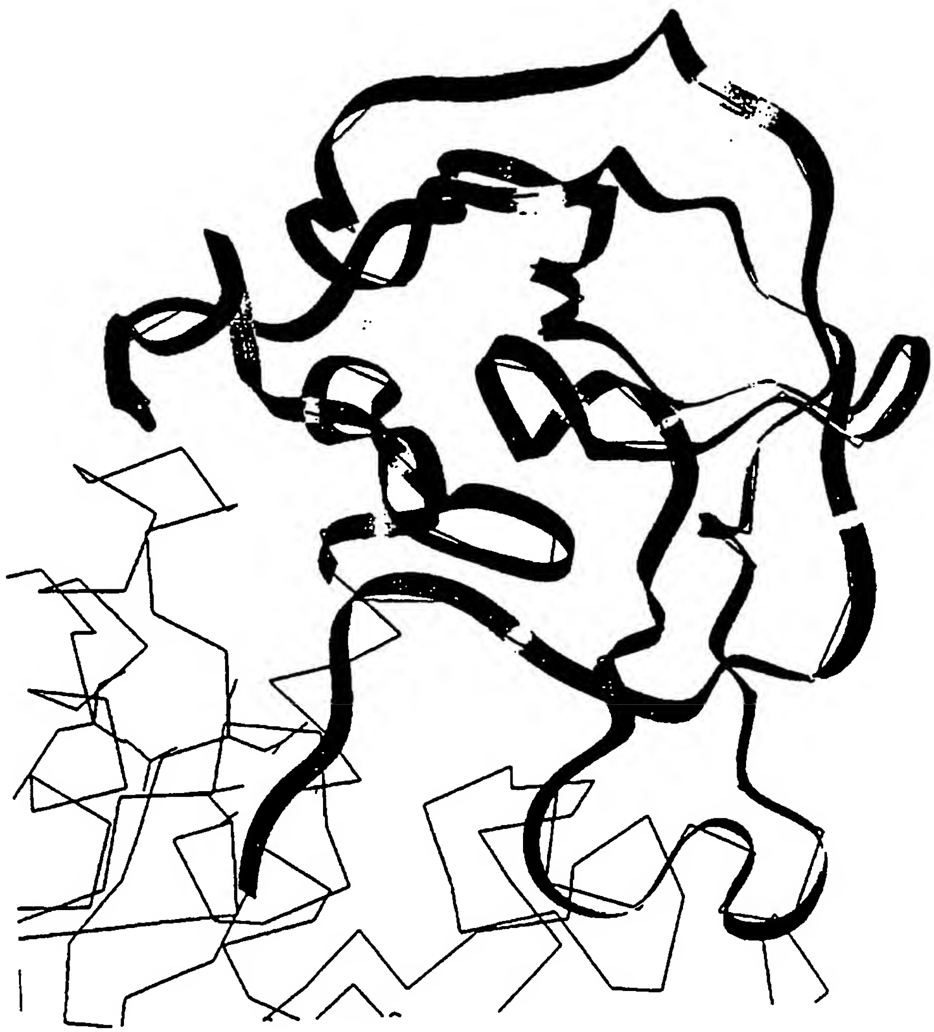

Fig. 7

8/11

1
CAT CAT AAT GGA ACA AAT GGT ACT ATG ATG CAA TAT TTC GAA TGG TAT TTG CCA AAT GAC
H H N G T N G T M M Q Y F E W Y L P N D

21
GGG AAT CAT TGG AAC AGG TTG AGG GAT GAC GCA GCT AAC TTA AAG AGT AAA GGG ATA ACA
G N H W N R L R D D A A N L K S K G I T

41
GCT GTA TGG ATC CCA CCT GCA TGG AAG GGG ACT TCC CAG AAT GAT GTA GGT TAT GGA GCC
A V W I P P A W K G T S Q N D V G Y G A

61
TAT GAT TTA TAT GAT CTT GGA GAG TTT AAC CAG AAG GGG ACG GTT CGT ACA AAA TAT GGA
Y D L Y D L G E F N Q K G T V R T K Y G

81
ACA CGC AAC CAG CTA CAG GCT GCG GTG ACC TCT TTA AAA AAT AAC GGC ATT CAG GTA TAT
T R N Q L Q A A V T S L K N N G I Q V Y

101
GGT GAT GTC GTC ATG AAT CAT AAA GGT GGA GCA GAT GGT ACG GAA ATT GTA AAT GCG GTA
G D V V M N H K G G A D G T E I V N A V

121
GAA GTG AAT CGG AGC AAC CGA AAC CAG GAA ACC TCA GGA GAG TAT GCA ATA GAA GCG TGG
E V N R S N R N Q E T S G E Y A I E A W

141
ACA AAG TTT GAT TTT CCT GGA AGA GGA AAT AAC CAT TCC AGC TTT AAG TGG CGC TGG TAT
T K F D F P G R G N N H S S F K W R W Y

161
CAT TTT GAT GGG ACA GAT TGG GAT CAG TCA CGC CAG CTT CAA AAC AAA ATA TAT AAA TTC
H F D G T D W D Q S R Q L Q N K I Y K F

181
AGG GGA ACA GGC AAG GCC TGG GAC TGG GAA GTC GAT ACA GAG AAT GGC AAC TAT GAC TAT
R G T G K A W D W E V D T E N G N Y D Y

201
CTT ATG TAT GCA GAC GTG GAT ATG GAT CAC CCA GAA GTA ATA CAT GAA CTT AGA AAC TGG
L M Y A D V D M D H P E V I H E L R N W

221
GGA GTG TGG TAT ACG AAT ACA CTG AAC CTT GAT GGA TTT AGA ATA GAT GCA GTG AAA CAT
G V W Y T N T L N L D G F R I D A V K H

241
ATA AAA TAT AGC TTT ACG AGA GAT TGG CTT ACA CAT GTG CGT AAC ACC ACA GGT AAA CCA
I K Y S F T R D W L T H V R N T T G K P

261
ATG TTT GCA GTG GCT GAG TTT TGG AAA AAT GAC CTT GGT GCA ATT GAA AAC TAT TTG AAT
M F A V A E F W K N D L G A I E N Y L N

281
AAA ACA AGT TGG AAT CAC TCG GTG TTT GAT GTT CCT CTC CAC TAT AAT TTG TAC AAT GCA
K T S W N H S V F D V P L H Y N L Y N A

Fig. 8

9/11

301
TCT AAT AGC GGT GGT TAT TAT GAT ATG AGA AAT ATT TTA AAT GGT TCT GTG GTG CAA AAA
S N S G G Y Y D M R N I L N G S V V Q K

321
CAT CCA ACA CAT GCC GTT ACT TTT GTT GAT AAC CAT GAT TCT CAG CCC GGG GAA GCA TTG
H P T H A V T F V D N H D S Q P G E A L

341
GAA TCC TTT GTT CAA CAA TGG TTT AAA CCA CTT GCA TAT GCA TTG GTT CTG ACA AGG GAA
E S F V Q Q W F K P L A Y A L V L T R E

361
CAA GGT TAT CCT TCC GTA TTT TAT GGG GAT TAC TAC GGT ATC CCA ACC CAT GGT GTT CCG
Q G Y P S V F Y G D Y Y G I P T H G V P

381
GCT ATG AAA TCT AAA ATA GAC CCT CTT CTG CAG GCA CGT CAA ACT TTT GCC TAT GGT ACG
A M K S K I D P L L Q A R Q T F A Y G T

401
CAG CAT GAT TAC TTT GAT CAT CAT GAT ATT ATC GGT TGG ACA AGA GAG GGA AAT AGC TCC
Q H D Y F D H H D I I G W T R E G N S S

421
CAT CCA AAT TCA GGC CTT GCC ACC ATT ATG TCA GAT GGT CCA GGT GGT AAC AAA TGG ATG
H P N S G L A T I M S D G P G G N K W M

441
TAT GTG GGG AAA AAT AAA GCG GGA CAA GTT TGG AGA GAT ATT ACC GGA AAT AGG ACA GGC
Y V G K N K A G Q V W R D I T G N R T G

261
ACC GTC ACA ATT AAT GCA GAC GGA TGG GGT AAT TTC TCT GTT AAT GGA GGG TCC GTT TCG
T V T I N A D G W G N F S V N G G S V S

481
GTT TGG GTG AAG CAA TAA
V W V K Q *

Fig. 8 (cont.)

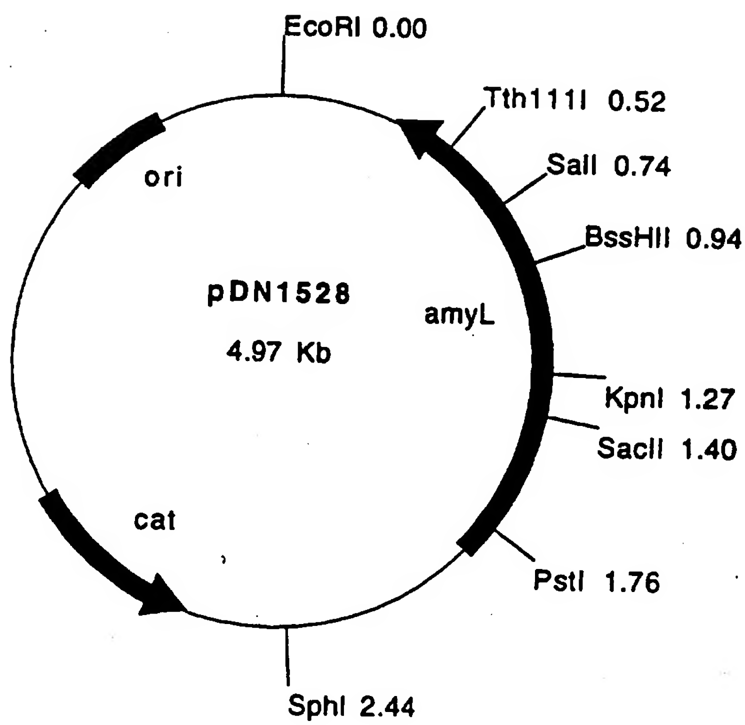
EcoRI 0.00
Tth111I 0.52
SalI 0.74
BssHII 0.94
KpnI 1.27
SacII 1.40
PstI 1.76
SphI 2.44
ori
amyL
cat
pDN1528
4.97 Kb

Fig. 9

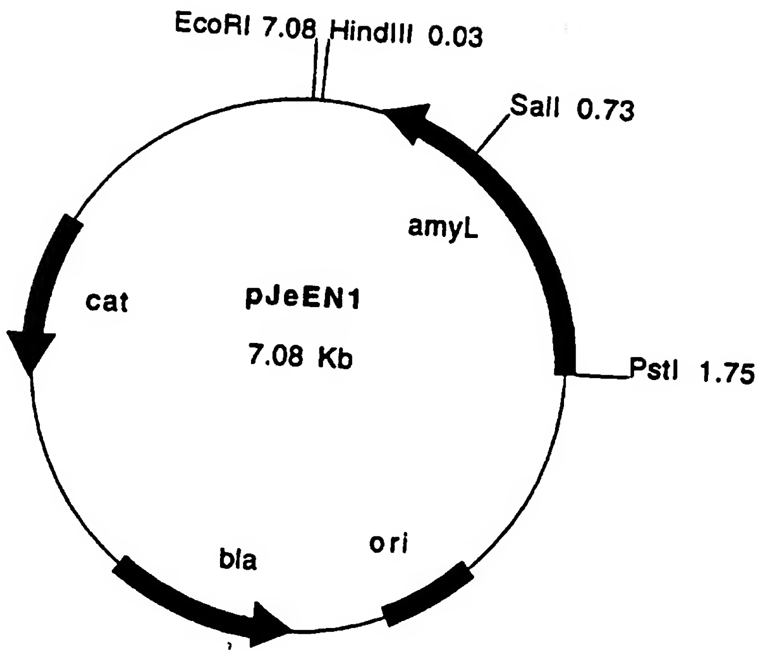
EcoRI 7.08
HindIII 0.03
SalI 0.73
amyL
cat
pJeEN1
7.08 Kb
PstI 1.75
bla
ori

Fig. 10

INTERNATIONAL SEARCH REPORT

International application No.
PCT/DK 96/00057

A. CLASSIFICATION OF SUBJECT MATTER

IPC6: C12N 9/28, C12N 15/56
According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

IPC6: C12N

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

SE,DK,FI,NO classes as above

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

WPI, CA, MEDLINE, BIOSIS

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
P,X	Dialog Information Services, File 5, BIOSIS PREVIEWS, Dialog accession no. 11619266, BIOSIS no. 98219266, Machius M et al: "Crystal structure of calcium-depleted Bacillus licheniformis alpha-amylase at 2.2 A resolution", & Journal of Molecular Biology 246 (4). 1995. 545-559 --	1-17
X	Dialog Information Services, file 155, MEDLINE, Dialog accession no. 08974640, MEDLINE accession no. 94289640, Svensson B: "Protein engineering in the alpha-amylase family: catalytic mechanism, substrate specificity, and stability", & Plant Mol Biol (NETHERLANDS) May 1994, 25 (2) p141-57 --	1-17

[X] Further documents are listed in the continuation of Box C. [X] See patent family annex.

* Special categories of cited documents:
"A" document defining the general state of the art which is not considered to be of particular relevance
"E" erlier document but published on or after the international filing date
"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)
"O" document referring to an oral disclosure, use, exhibition or other means
"P" document published prior to the international filing date but later than the priority date claimed
"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
"X" document of particular relevance: the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
"Y" document of particular relevance: the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art
"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
5 July 1996	05 -07- 1996
Name and mailing address of the ISA/ Swedish Patent Office Box 5055, S-102 42 STOCKHOLM Facsimile No. +46 8 666 02 86	Authorized officer Yvonne Siösteen Telephone No. +46 8 782 25 00

INVITATION TO PAY ADDITIONAL FEES

International application No.

PCT/DK 96/00057

The invention claimed relates to a method of constructing alpha-amylase variants with predetermined properties by comparing the three-dimensional structures of enzymes. The claims also include many alpha-amylase variants.

"A search for a special technical feature" as mentioned in PCT Rule 13.2 among the independent claims did not reveal a unifying, novel technical feature.

Accordingly, the following inventions were found:

I Claims 1-17 focus on a method of constructing alpha-amylase variants by comparing the tree-dimensional structure of a parent enzyme (Temamyl-like alpha-amylase) with another enzyme e.g. mammalie or fungal alpha-amylases. The differences in structure are compared with the differences in function, whereafter new variants with new predictable characteristics are produced.

II Claims 45-46 directed to a alpha-amylase variant that has decreased Ca2+ dependency,

III Claim 47 directed to a alpha-amylase variant that exhibits higher activity below the ph-optimum than the parent enzyme.

IV Claim 48 directed to a alpha-amylase variant having an increased thermostability and/or altered temperature optimum.

V Claim 50 directed to a variant having reduced capability of cleaving an oligo-saccharide substrate close to its branching point.

Due to the complex construction of the claims and the fact that the search so far has not covered all aspects of the invention, it may be that further non-unity remarks can appear. If further searches are done, references might appear which will give furter a posteriori non-unity remarks.

Therefore, the search has been restricted to the first invention.

Claims 18-43 are directed to a number of different variants that are composed of several inventions. They are, however, so complex and broad that no meaningful search can be done, especially as no special characteristic is linked to the groups of variants. It is for example unlikely that claim 18 concerns one invention. It is not believable that a change in any amino acid in one fragment for one/or none of the amino acids in a fragment of another enzyme gives an enzyme with the same new and valuable characteristic. The formulation of claims 18-43 is so complicated because of all the different combinations of amino acid substitutions.

Thus they do not comply with Art. 6. PCT prescribing that claims shall be clear and concise.

INTERNATIONAL SEARCH REPORT

International application No.
PCT/DK 96/00057

C (Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	Dialog Information Services, file 155, MEDLINE. Dialog accession no. 08958150, MEDLINE accession no. 94273150, Nakatani H et al: "Effect of modifying histidine residues on the action of Bacillus amyloliquefaciens and barley-malt alpha-amylases", & Carbohydr Res (NETHERLANDS) Apr 16 1994, 257 (1) p 155-61	1-17
Y		45-46
	--	
X	J. MED. BIOL., Volume 229, 1993, C. Chang et al, "Crystallization and Preliminary X-ray Crystallographic Analysis of alpha-Amylase from Bacillus subtilis" page 235 - page 238	1-17
	--	
A	WO 9100343 A2 (GIST-BROCADES N.V.), 10 January 1991 (10.01.91)	1-17
	--	
A	EP 0410498 A2 (GIST-BROCADES N.V.), 30 January 1991 (30.01.91)	1-17
	--	
A	JOURNAL OF BACTERIOLOGY, Volume 166, No 2, May 1986, G. L. Gray et al, "Structural Genes Encoding the Thermophilic alpha-Amylases of Bacillus stearothermophilus and Bacillus licheniformis" page 635 - page 643	1-17
	--	
P,X	WO 9535382 A2 (GISTBROCADES B.V.), 28 December 1995 (28.12.95), claims 1-2, abstract	45-46
	--	
Y	WO 9418314 A1 (GENENCOR INTERNATIONAL), 18 August 1994 (18.08.94)	45-46
	--	

INTERNATIONAL SEARCH REPORT

International application No.
PCT/DK 96/00057

C (Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	Chemical Abstracts, Volume 108, No 11, 14 March 1988 (14.03.88), (Columbus, Ohio, USA), Buisson, G. et al, "Three dimensional structure of porcine pancreatic alpha-amylase at 2.9 Å resolution. Role of calcium in structure and activity", page 325, THE ABSTRACT No 90927h, EMBO J. 1987, 6 (13), 3909-3916 --	45-46
Y	Chemical Abstracts, Volume 112, No 15, 9 April 1990 (09.04.90), (Columbus, Ohio, USA), Vihinen, Mauno et al, "Site-directed mutagenesis of a thermostable alpha-amylase from Bacillus stearothermophilus: putative role of three conserved residues", page 347, THE ABSTRACT No 135178r, J. Biochem 1990, 107 (2), 267-272 --	45-46
A	US 4600693 A (KAREN L. KINDLE ET AL), 15 July 1986 (15.07.86) --	45-46
A	Chemical Abstracts, Volume 112, No 19, 7 May 1990 (07.05.90), (Columbus, Ohio, USA), Holm, Liisa et al, "Random mutagenesis used to probe the structure and function of Bacillus stearothermophilus alpha-amylase", page 351, THE ABSTRACT No 174785f, Protein Eng. 1990, 3 (3), 181-191 -- --------	45-46

INTERNATIONAL SEARCH REPORT

International application No.
PCT/DK96/00057

Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)

This international search report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claims Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:

2. ☒ Claims Nos.:
because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:

see next sheet

3. ☐ Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

see next sheet

1. ☐ As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.

2. ☐ As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.

3. ☒ As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.:
Claims 1-17 directed to a method of constructing alpha-amylase variants and claims 45-46 directed to an alpha-amylase.

4. ☐ No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

Remark on Protest
☐ The additional search fees were accompanied by the applicant's protest.
☒ No protest accompanied the payment of additional search fees.

INTERNATIONAL SEARCH REPORT
Information on patent family members

01/04/96

International application No.
PCT/DK 96/00057

Patent document cited in search report		Publication date	Patent family member(s)		Publication date
WO-A2-	9100343	10/01/91	AU-B,B-	629959	15/10/92
			AU-A-	5939790	17/01/91
			CA-A-	2032518	30/12/90
			EP-A,A,A	0409299	23/01/91
			JP-T-	4500609	06/02/92
EP-A2-	0410498	30/01/91	AU-B-	638263	24/06/93
			AU-A-	5953890	17/01/91
			CA-A-	2030554	30/12/90
			CN-A-	1050220	27/03/91
			JP-T-	4500756	13/02/92
			US-A-	5364782	15/11/94
			WO-A,A,A	9100353	10/01/91
WO-A2-	9535382	28/12/95	NONE		
WO-A1-	9418314	18/08/94	NONE		
US-A-	4600693	15/07/86	NONE		